ground water

# Optimizing Remediation of an Unconfined Aquifer Using a Hybrid Algorithm

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## Abstract

We present a novel hybrid algorithm, integrating a genetic algorithm (GA) and constrained differential dynamic programming (CDDP), to achieve remediation planning for an unconfined aquifer. The objective function includes both fixed and dynamic operation costs. GA determines the primary structure of the proposed algorithm, and a chromosome therein implemented by a series of binary digits represents a potential network design. The time-varying optimal operation cost associated with the network design is computed by the CDDP, in which is embedded a numerical transport model. Several computational approaches, including a chromosome bookkeeping procedure, are implemented to alleviate computational loading. Additionally, case studies that involve fixed and time-varying operating costs for confined and unconfined aquifers, respectively, are discussed to elucidate the effectiveness of the proposed algorithm. Simulation results indicate that the fixed costs markedly affect the optimal design, including the number and locations of the wells. Furthermore, the solution obtained using the confined approximation for an unconfined aquifer may be infeasible, as determined by an unconfined simulation.


## Introduction

Unconfined aquifers lack an upper confining layer and are near the ground surface. Thus, contamination from surface sources is more likely to occur in an unconfined aquifer than in a confined one. However, most earlier studies of ground water remediation dealt with confined aquifers (Chang et al. 1992; Ritzel et al. 1994; McKinney and Lin 1995; Bear and Sun 1998; Hilton and Culver 2000). This limitation probably follows from the fact that the flow equation for an unconfined aquifer is nonlinear and is more complex than that for a confined aquifer. Recently, Mansfield and Shoemaker (1999) implemented a successive approximation linear quadratic regulator algorithm (SALQR, Chang et al. 1992) to obtain least-cost pump-and-treat remediation policies for cleaning up unconfined aquifers. Their study derived and computed the analytic derivatives of the nonlinear unconfined aquifer flow and transport equations. However, Mansfield and Shoemaker (1999) did not consider the fixed costs of well installation.

Pump-and-treat systems are the most common remedial systems for restoring contaminated aquifers (Gorelick et al. 1984; Ahlfeld et al. 1988; Andricevic and Kitanidis 1990; Yeh 1992). Evaluating the decision variables typically requires determining pumping rates from extraction wells and selecting the locations of the wells. Mathematical programming is commonly simplified by ignoring the fixed costs of well installation due to discontinuities in selecting well locations. The optimal network commonly includes wells whose final, optimized pumping rates are nonzero. However, this simplification can result in designs that depend on pumping numerous wells at low rates over long periods (McKinney and Lin 1995). Various methodologies for incorporating these fixed costs have recently attracted increasing interest. McKinney and Lin (1994, 1995) considered both fixed and operating costs in the objective function and applied genetic algorithms (GAs) and mixed-integer nonlinear programming (MINLP) to solve the problem; they considered only constant pumping rates and a steady-state ground water system. Watkins and McKinney (1998) employed generalized Benders decomposition and outer approximation to water resource problems that involve

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cost functions with both discrete and nonlinear terms. Their algorithms suffer from a computational bottleneck for large MINLP problems, such as ground water remediation planning with time-varying pumping rates. Zheng and Wang (1999) integrated tabu search and linear programming to design remediation strategies, accounting for both fixed and operating costs. They take advantage of the fact that the global optimization approach is most effective for optimizing discrete well location variables, while linear programming is much more efficient for optimizing continuous pumping rate variables.

Unlike the static algorithms of linear or nonlinear programming, optimal-control algorithms efficiently solve dynamic control problems such as remediation planning with time-varying pumping rates. By applying the SALQR, Chang et al. (1992) demonstrated that dynamic pumping policies are more cost effective than the best static pumping policies because pumping rates are allowed to vary as the contaminant plume moves (Chang et al. 1992; Culver and Shoemaker 1992). Culver and Shoemaker (1993) extended the SALQR method by adding second derivatives as governed by a quasi-Newtonian approach (QNDDP), accelerating the convergence of the algorithm. Culver and Shoemaker (1997) employed the QNDDP algorithm to solve a ground water reclamation problem by assuming that the capital cost of treatment was linearly related to the extraction rate. However, none of the aforementioned studies considered the fixed cost of installing wells. One difficulty associated with applying the optimal control–based algorithms to a problem while considering the fixed cost is that the optimal-control theory requires the problem to be separable in each time step. Yet, the problem is nonseparable when the objective function includes the fixed cost. Another difficulty related to the fixed cost is that this cost depends on the number and locations of wells. Consequently, the objective function is nondifferentiable when the fixed cost is included. However, differential dynamic programming requires that objective and transfer functions are differentiable.

Combinatory algorithms such as GA, simulated annealing, and tabu search have been extensively applied to problems of ground water management (Dougherty and Marryott 1991; McKinney and Lin 1994; Ritzel et al. 1994; Rizzo and Dougherty 1996; Huang and Mayer 1997; Wang and Zheng 1998; Aly and Peralta 1999; Zheng and Wang 1999). Huang and Mayer (1997) employed GA to search for the optimal pumping rates and the discrete spaces of well locations in dynamic ground water remediation management. Their findings reveal that solutions obtained using the moving-well model are less expensive than those obtained using a comparable fixed-well model. Their model requires considerable computational effort to yield the optimal solution because of the characteristics of the GA. Wang and Zheng (1998) used a GA and simulated annealing, coupled with MODFLOW, to solve the ground water remediation design problem with multiple management periods and an objective function that involved both fixed and operating costs. However, their study limited the maximum number of planning periods to four, probably because the computational expense of GAs and simulated annealing increases rapidly with the number of planning periods and corresponding decision variables. Aly and Peralta (1999) used the $L_\infty$ norm as a global measure of aquifer contamination, instead of considering contaminant concentrations at traditional control locations, and compared the performance of a GA to that of MINLP. Rizzo and Dougherty (1996) solved a large-scale, six-management-period problem, using simulated annealing. Although their model can be applied to a dynamic system and incorporates fixed and operating costs, the multiperiod planning problem must be approximated by a series of single-period problems. Accordingly, their approach is not a fully dynamic optimization method. Despite the fact that the combinatory algorithms can solve the problem of discontinuity associated with the fixed cost, the algorithm cannot be efficiently applied to a dynamic system since the computational effort increases significantly with the number of decision variables because the time step increases.

The GA is appealing since it does not require the objective function to be differentiable. It can thus easily incorporate the fixed costs associated with ground water remediation. However, applying only this method to solve time-varying policies would drastically increase the computational resources required. This investigation, therefore, proposes a novel approach to solving such an optimization problem by effectively combining a GA with constrained differential dynamic programming (CDDP) in which a ground water simulator is embedded.

## Transition Equation

Based on the Dupuit assumption, the vertically integrated two-dimensional equation for ground water flow and transport of a conservative solute with adsorption in an unconfined aquifer is expressed as follows.

$$\nabla K h \nabla h \pm \sum_{i \in I} u_i \delta(x_i, y_i) = S_y \frac{\partial h}{\partial t} \tag{1}$$

$$\nabla(\theta h D \nabla c) - \nabla(h \theta v c) - \sum_{i \in I} u_i (c - c') \delta(x_i, y_i) = \frac{\partial}{\partial t}(R h \theta c) \tag{2}$$

where $h$ is the hydraulic head; $K$, the hydraulic conductivity; $I$, an index set that defines the feasible well locations in the aquifer; $u_i$, the flow rate of a pumping well at point $(x_i, y_i)$; $\delta(\cdot)$, a Dirac delta function; $S_y$, the specific yield; $c$, the concentration; $v$, Darcy's velocity; $\theta$, the porosity; $R$, the retardation coefficient; and $D$, the hydrodynamic dispersion tensor. Equations 1 and 2 are nonlinear and are subject to appropriate initial and boundary conditions. The equations are solved using Galerkin's finite-element method and the implicit finite-difference scheme. The resulting matrix equations can be expressed as follows (Mansfield and Shoemaker 1999).

$$\left([A]_{h_{t+1}} + \frac{[B]}{\Delta t}\right)\{h_{t+1}\} = \frac{[B]}{\Delta t}\{h_t\} - \{f_{h,t}\} + \left[L_h\right]\{u_t\} \tag{3}$$

$$\left([N]_{h_{t+1}}+\frac{[M]_{h_{t+1}}}{\Delta t}\right)\{c_{t+1}\}=\frac{[M]_{h_{t+1}}}{\Delta t}\{c_t\}-\{f_{c,t}\}+[L_c(u_t)]\{c'-c_{t+1}\} \quad (4)$$

Mansfield and Shoemaker (1999, p. 1457) completely detailed the matrix terms in Equations 3 and 4, which contain information on the spatial distribution of the physical parameters that relate to flow and transport in the aquifer. Here, the unconfined aquifer simulator is modified from the ISOQUA (Pinder 1978), a two-dimensional confined aquifer simulator, using the Picard method. Given that $n_h$ and $n_c$ are non-Dirichlet nodes associated with head ($h_t$) and concentration ($c_t$,), respectively, the hydraulic head and concentration in an aquifer model are real vectors with dimensions $n_h$ and $n_c$, respectively. The state vector $x_t$ combines $h_t$ and $c_t$, as expressed in $x_t = \langle h_t : c_t \rangle^T \in R^{(n_h+n_c)\times 1}$. Using this notation, Equations 3 and 4 can be combined to yield the change of the state between time steps as the transition equation $\{x_{t+1}\} = T(x_t u_t)$.

## Model Formulation

Typically, a ground water remediation design problem involves three types of decision variables (Zheng and Wang 1999): the number of required extraction wells, the locations where the wells should be installed, and the rates at which the water should be pumped after the well locations have been determined. The proposed remediation planning model involves all three types of decision variables. The proposed model seeks to minimize the total remediation cost using pump and treat for an unconfined aquifer. The remediation cost includes the fixed costs of installing the wells and the operating costs associated with the time-varying pumping rates. The planning model of the unconfined aquifer remediation can be formulated as

$$\min_{\substack{I\subset\Omega \\ u_t^i, i\in I, t=1,\dots,N}} \quad J=\sum_{i\in I}\left\{a_1 y^i(I) + \sum_{t=1}^{N}\left[a_2 u_t^i(I)+a_3 u_t^i(I)\left[L_*^i(I)-h_{t+1}^i(I)\right]\right]\right\} \quad (5)$$

subject to

$$\{x_{t+1}\} = \mathrm{T}(x_t, u_t(I)), \quad t = 1,2,\dots,N, \quad I\subset\Omega \quad (6)$$

$$c_{N,j} \le c_{\max}, \quad j \in \Phi \quad (7)$$

$$\sum_{i\in I} u_t^i \le d_{\max}, \quad t = 1,2,\dots,N \quad (8)$$

$$u_{\min}^i \le u_t^i(I) \le u_{\max}^i, \quad t = 1,2,\dots,N, \quad I\subset\Omega \quad (9)$$

where $\Omega$ is a set of indexes that defines all the candidate locations of wells within the aquifer, and $I$ is a subset of $\Omega$, a possible network alternative, and is represented by a chromosome in the GA. The upper index, $i$, denotes a single well in the network alternative, $I$. $\Phi$ represents the set of observation wells. Equation 5 gives the total cost, which depends on the network alternatives, $I$ and the associated pumping policy ($u_t(I)$, $t = 1, \dots, T$). $x_{t+1}$ is the state vector at time $t + 1$. $a_1$, $a_2$, and $a_3$ are coefficients used to convert the well installation cost, the treatment cost, and the operating cost, respectively, into monetary values ($). $y^i(I)$ equals the depth of each well in a network design. $L_*^i(I)$ is the distance between the ground surface and the lower datum of the aquifer for each well. $u_t^i(I)$ is the variable pumping rate at time $t$, and $h_{t+1}^i(I)$ denotes the hydraulic head for each node at time $t + 1$. The expression $L_*^i(I)-h_{t+1}^i(I)$ represents drawdown at pumping well $i$. Equation 7 specifies the water quality standard at the end of the planning period. $c_{\max}$ is the maximum allowable concentration of contaminants. $d_{\max}$ represents the maximum allowable total pumping rate from all extraction wells. Equation 9 specifies the capacity constraints on each well.

The objective function of the total cost given by Equation 5 is mixed integer and nonlinear. Thus, the ground water remediation model defined by Equations 5 to 9 represents a mixed-integer, time-varying optimization problem. The first term in Equation 5 is the cost of installing a well for pumping. The installations of wells are discrete operations that depend on binary variables in the optimization model. The second term in Equation 5 is the operating cost, which includes the pumping and treatment costs (Chang et al. 1992; Culver and Shoemaker 1992). These costs are continuous functions of the state and control variables and are separable functions in each time stage, $t$. In contrast, the fixed cost indicated by the first component is nonseparable. The problem, defined by Equations 5 to 9, cannot be easily solved using only CDDP because the installation cost is discrete and nonseparable. However, using only GA to determine time-varying policies would dramatically increase the computational resources required (Culver and Shoemaker 1997; Zheng and Wang 1999).

## Computational Algorithm

No optimization method exists for solving the problem defined by Equations 5 to 9, so a hybrid algorithm, integrating GA and CDDP (GCDDP), is proposed herein. In this integrated approach, GA is used to find the optimal network design, including the number and locations of wells, while CDDP is used to calculate the optimal pumping policy associated with each network design. GA is a heuristic, probabilistic, search-based optimization technique for searching a solution space to identify the best solution. A solution determined using a GA is not necessarily optimal but is merely the best identified solution. GA sets an initial population using a uniform random number generator and propagates this initial population through $K$ generations. Propagating from $(k - 1)$ to $k$ ($k$ = generation index), GA performs three operations—selection, crossover, and mutation. GA generates a new population of equal size by selecting strings with higher fitness values with higher probabilities. GA perturbs the resulting population by applying a crossover with a probability of $p_c$ and then perturbs it further by performing mutation with probability $p_m$. Tournament selection and one-point crossover are employed here. Hsiao and Chang (2002) present the method of integrating GA and CDDP. In this study, we follow the procedures of their work and discuss some issues as follows.

### Encoding and Decoding Chromosomes

GA uses a binary string (also referred to as a chromosome) to encode a trial solution; the string comprises numerous binary bits. In this investigation, a binary representation is mapped to real-world locations of wells; each bit in a chromosome is associated with a candidate site, and the length of the chromosome equals the total number of candidate sites available for installing wells. If the value of a bit is 1, then a well will be installed at the associated candidate site; otherwise, the value of a bit is 0, and no well is installed. A hypothetical, homogeneous, isotropic, unconfined 600- × 1200-m aquifer is considered to demonstrate the encoding of chromosomes. Ninety-one nodes, 24 candidate well sites, and 17 observation wells are included in the finite-element mesh (Figure 1). This investigation assumes that the optimal network is symmetrical, just as the hydraulic head, the initial concentration, the locations of the observation wells, and candidate sites for the pumping wells are symmetrical. This assumption reduces the number of combinations of network configurations in GA and the computational effort. The chromosome contains 16 bits, of which the first 8 represent sites along the centerline and the final 8 represent candidate sites in the upper region. One of the last eight bits with a value represents two wells placed symmetrically about the centerline. The chromosome can be easily encoded and decoded since the well selection is binary.

### Evaluating the Fitness of Each Chromosome

Most of the computational loading of the proposed algorithm is concentrated in evaluating the fitness. The model defined by Equations 5 to 9 is divided into the following two levels of problems to facilitate the application of GCDDP.

Main problem:

$$\min_{I \subset \Omega} J_1(I) = \sum_{i \in I} \left[ a_1 y_*^i + J_2^*(I) \right] \tag{10}$$

Sub problem:

$$J_2^*(I) = \min_{u_t(I), t=1,\ldots,T} \sum_{t=1}^{T} \left\{ a_2 l^{\mathrm{T}} u_t(I) + a_3 u_t(I) \left[ L_*(I) - h_{t+1}(I) \right] \right\} \tag{11}$$

$$\text{subject to Equations 6 to 9} \tag{12}$$

GA solves the main problem, and the objective function contains the installation of wells and optimal time-varying costs. The optimal operating costs for each chromosome are the solution to the subproblem, determined by CDDP. In executing the algorithm the pumping rate is treated as fixed in the GA step and the well location is assumed to be fixed in the CDDP algorithm (Figure 2). Therefore, this algorithm is a simple GA with embedded CDDP to compute the optimal operating costs for a potential network alternative (represented by a chromosome). The CDDP used herein modifies the SALQR algorithm (Chang et al. 1992). The SALQR algorithm incorporates the water quality and extraction constraints (Equations 7 to 9 into Equation 11) to solve the optimization problem as an unconstrained one. This study employs a penalty function to consider the water quality constraints described by Equation 7 and applies quadratic programming (Murray and Yakowitz 1979) at each stage in the backward and forward sweep of CDDP to handle the control constraints

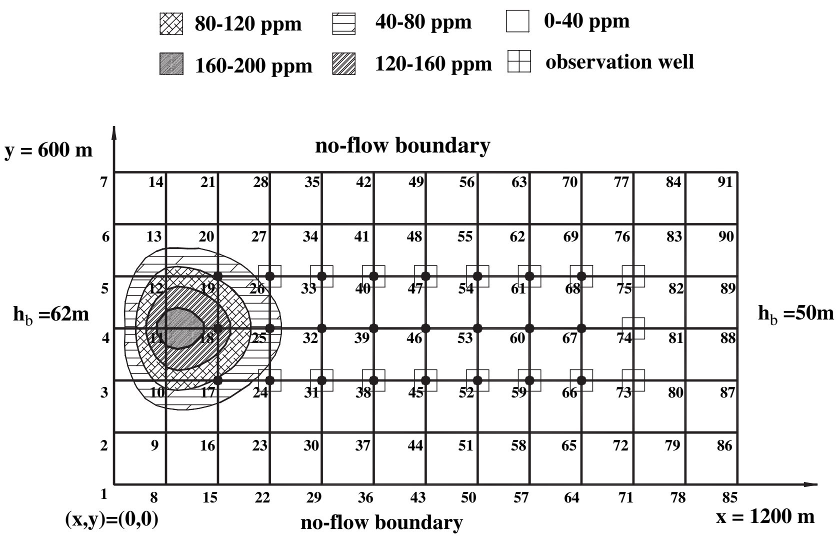


**Figure 1. Finite-element mesh, boundary conditions, initial plume, and locations of numbered observations and potential extraction wells for all runs of the ground water reclamation example.**

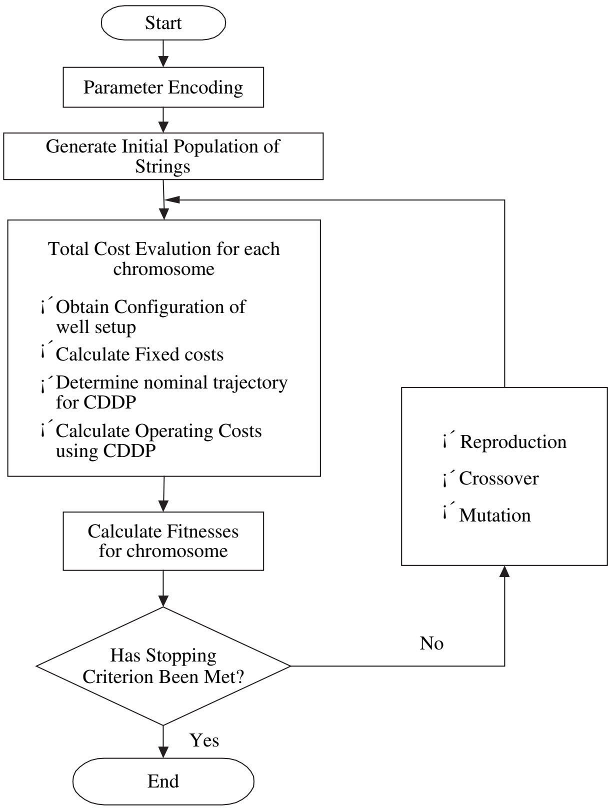


**Figure 2. Flowchart for integrating GA and CDDP.**

represented by Equations 8 and 9. The penalty function can be found in Lin (1990) and is expressed as follows.

$$p_k(f_k) = \xi_k, \quad \xi_k \le 1 \tag{13}$$

$$p_k(f_k) = c_1\xi_k^2 + c_2\xi_k^{1/2} + c_3 \quad \xi_k > 1 \tag{14}$$

with

$$\xi_k = (w_k^2 f_k^2 + \epsilon_k^2)^{1/2} + w_k f_k \tag{15}$$

where $w_k$ is the weighting coefficient of the $k$th constraint; $\varepsilon_k$, is a shape parameter of the hyperbolic function $\xi_k$, and $c_1$, $c_2$, and $c_3$ are constant coefficients. Chang et al. (1992) demonstrated that this penalty function is numerically efficient; Culver and Shoemaker (1992, 1993, 1997) and Mansfield and Shoemaker (1999) subsequently applied it. Since it is a derivative-based algorithm, CDDP takes the first derivatives of the transition equations (simulation models), the objective function, and the constraints (Equation 7) with respect to the state and control variables. Of these derivatives, those of the transition equations are the most complex. Fortunately, Mansfield and Shoemaker (1999) derived the analytic derivatives of transition functions (Equations 3 and 4), but equations 16, 17, and 19 in their paper included some typographical errors, which are corrected as follows.

$$\frac{\partial c_{t+1}}{\partial h_t} = \left([N]_{t+1} + \frac{[M]_{t+1}}{\Delta t} + L_c(u_t)\right)^{-1} \times \left([S]_{t+1} - [R]_{t+1} - [W]_{t+1}\right)\left[\frac{\partial h_{t+1}}{\partial h_t}\right] \tag{16}$$

$$\frac{\partial c_{t+1}}{\partial c_t} = \left([N]_{t+1} + \frac{[M]_{t+1}}{\Delta t} + L_c(u_t)\right)^{-1} \frac{[M]_{t+1}}{\Delta t} \tag{17}$$

$$\frac{\partial c_{t+1}}{\partial u_t} = \left([N]_{t+1} + \frac{[M]_{t+1}}{\Delta t} + L_c(u_t)\right)^{-1} \times \left([S]_{t+1} - [R]_{t+1} - [W]_{t+1}\right)\left[\frac{\partial h_{t+1}}{\partial u_t}\right] \tag{18}$$

Mansfield and Shoemaker (1999, p. 1459) completely defined the terms, $[S]_{t+1}$, $[R]_{t+1}$, and $[W]_{t+1}$. GCDDP requires recalculating the problem defined by Equations 11 and 12, greatly increasing the total computational effort. Decreasing the computational effort of CDDP substantially reduces the total central processing unit (CPU) requirement. This investigation, therefore, applies the sparse structure of the derivative equations of state transition, developed by Mansfield et al. (1998), to reduce the computational effort of the CDDP. Moreover, each CDDP calculation can be performed according to only an initial nominal policy. Therefore, a systematic procedure must be performed to yield an initial nominal policy associated with each chromosome. All pumping wells are assumed to have pumping rates 0.1 $m^3/s$ as an initial nominal policy for all chromosomes.

### Termination Criterion

The GA is computed in consecutive generations for which the termination criterion is heuristic. The algorithm is ended when the fitness of the optimal chromosome remains constant over 10 generations or the number of generations exceeds a given maximum. The fitness of a chromosome is a function of its optimal total cost. A higher total cost corresponds to a lower fitness.

## Numerical Results

Two examples are provided to investigate the feasibility of applying GCDDP to solve unconfined aquifer remediation problems. These examples involve constant unit fixed costs and unit fixed costs that vary with geological conditions. The design of an unconfined aquifer using an unconfined model is compared with that using an approximate confined model. Using an unconfined simulator to review the design generated by the approximate confined model reveals that the design may not be feasible.

The aquifer (Figure 1) is modified from the example of Chang et al. (1992) and Culver and Shoemaker (1997). The hydraulic head distribution before pumping is assumed to be steady; the initial peak concentration within the aquifer is 200 mg/L, and the water quality at the end of 5 years must be <0.5 mg/L at all the observation wells. The period between each stage in the management model is 91.25 d. Table 1 describes the characteristics of the aquifer. The coefficients $a_1$, $a_2$, and $a_3$ are all constants (Table 2). The performance of all examples depends on the appropriate setting of the crossover probability ($p_{\mathrm{cross}}$), the population size, and the mutation probability ($p_{\mathrm{mutant}}$). Numerical experiments in which the unit fixed

**Table 1**
**Aquifer Properties for the Example Application**

| Parameter | Unconfined Aquifer | Confined Aquifer |
|---|---|---|
| Hydraulic conductivity (m/s) | $5.79 \times 10^{-4}$ | $5.79 \times 10^{-4}$ |
| Longitudinal dispersivity (m) | 21.3 | 21.3 |
| Transverse dispersivity (m) | 2.13 | 2.13 |
| Diffusion coefficient ($m^2$/s) | $1 \times 10^{-7}$ | $1 \times 10^{-7}$ |
| Storage coefficient | 0.1 | 0.001 |
| Porosity | 0.2 | 0.2 |
| Sorption partitioning coefficient ($cm^3$/g) | 0.245 | 0.245 |
| Media bulk density (g/$cm^3$) | 2.12 | 2.12 |
| Aquifer thickness $b$ (m) | 50 | 50 |
| Distance from ground surface to lower datum $L_*$ (m) | 120 | 120 |

cost ($a_1$) is \$240/m are performed to examine the sensitivity of GA's parameters to $p_{\text{cross}}$ from 0.5 to 0.8, to the population size from 60 to 90, and to $p_{\text{mutant}}$ = 1/population (adapted from the suggestion of DeJong 1975). The results (Table 3) indicate that within the specified ranges, the parameters minimally affect the optimal values. Consequently, the solutions in the following examples are obtained when $p_{\text{cross}}$ is 0.8 and the population has a size of 70 chromosomes.

## Constant Fixed Costs

This section addresses a case that examines the effect of fixed cost on the optimal total cost and the network design for an unconfined aquifer. The solutions to the unconfined aquifer remediation problem with constant unit fixed costs (Table 4) show that the number of wells decreases as the unit fixed cost increases from \$0 to \$240/m. The operating costs increase with the unit fixed cost. The optimal design involves seven wells when the fixed cost is zero and two wells when the unit fixed cost is \$240/m. The results are reasonable because a design with more wells more efficiently distributes the required pumping rates across the wells, reducing the total drawdown and the operating costs. The minimum total pumping volume of the wells is 39.74 L/s simulation period in the case of zero fixed cost and 583.17 L/s · simulation period when the unit fixed cost is \$240/m. This result confirms that an optimal design tends to include wells that pump at low rates if the fixed cost is neglected. Table 4 shows the required CPU time and number of generations to convergence. The examples are run on a PC with an AMD Athlon™ 1000 MHz CPU.

**Table 2**
**Cost Function Coefficients for the Example Problem**

| Coefficient | Value |
|---|---|
| $a_1$ | \$0 to \$240/m |
| $a_2$ | \$40,000 ($m^3$/s simulation period) |
| $a_3$ | \$1000 ($m^3$/s simulation period) |

**Table 3**
**Sensitivity Analysis of the Parameters for the Unconfined Aquifer Model with Unit Fixed Cost of \$240/m**

| Population Size | OV | | | |
|---|---|---|---|---|
| | $P_{\text{cross}} = 0.5$ | $P_{\text{cross}} = 0.6$ | $P_{\text{cross}} = 0.7$ | $P_{\text{cross}} = 0.8$ |
| 60 | 273 | 307 | 270 | 270 |
| 70 | 261 | 270 | 261 | 261 |
| 80 | 273 | 273 | 270 | 261 |
| 90 | 261 | 278 | 278 | 270 |

$P_{\text{cross}}$ = crossover probability; OV = the computed optimal objective function (divided by 1000).

For comparison, the total cost of the design with zero fixed cost is evaluated by adding the calculated operating costs to the fixed costs that are estimated by multiplying the well depth by the unit fixed cost. The total cost of the design with no fixed cost is 47.24% higher than that of the design with fixed costs, which is \$240.0/m (Table 5). Accordingly, a significant total cost saving can be realized by applying the novel GCDDP algorithm and considering the fixed cost in the design process.

Using the optimal network design and pollutant concentration distribution at the end of the planning period in cases in which the unit fixed cost is \$60.0 and \$240/m, it is clear that as the plume moves from west to east, the pumping wells in the western region are better able to remove the contaminant (Figure 3). The hydraulic head of the western region is higher than that of the eastern region. Therefore, the pumping cost of the former well is lower. Consequently, pumping wells with uniform unit fixed costs (Figure 3) are more likely to be situated in the west.

## Comparison of Design Using an Unconfined and a Confined Model

This section examines the discrepancy of the network design generated using the embedded confined transition equation for an unconfined aquifer. The nonlinearity of the unconfined transition equation complicates

**Table 4**
**Optimal Solutions for the GCDDP with Uniform Unit Fixed Costs**

| Fixed Unit Costs | \$0/m | \$60/m | \$240/m |
|---|---|---|---|
| No. of wells | 7 | 3 | 2 |
| Total operating cost | 183,107 | 187,115 | 203,671 |
| Minimum total pumping volume (L/s simulation period) | 39.74 | 312.21 | 583.17 |
| Number of generation | 14 | 15 | 16 |
| CPU time required (s) | 185,916 | 142,934 | 158,384 |

**Table 5**
**Total Cost Comparison with/without Unit Fixed Costs in an Optimization Model**

| Coefficient $a_1$ | \$60.0/m | \$240/m |
|---|---|---|
| Total cost for the network designed without fixed costs ($J_1$) | 233,507 (seven wells) | 384,707 (seven wells) |
| Total cost for the networks designed with fixed costs ($J_2$) | 208,715 (three wells) | 261,271 (two wells) |
| Ratio of difference (($J_1 - J_2$)/$J_2$) (%) | 11.88 | 47.24 |

the simulation and the associated calculation on which the CDDP algorithm depends. Therefore, an approximate confined transition equation is commonly embedded into the management model to simulate the ground water flow and contaminant transport of an unconfined aquifer in order to simplify the computation. However, this approximation can generate a situation in which the optimal design, including the pumping rates obtained using an embedded confined transition equation, fails to meet concentration constraints according to an unconfined simulation model. The comparison is made as follows.

1. An unconfined aquifer remediation problem is solved using the embedded unconfined transition equation.
2. An unconfined aquifer remediation problem is solved using the embedded confined transition equation, wherein the initial hydraulic head of the unconfined aquifer is applied as the thickness of the confined simulator.
3. An unconfined aquifer simulation is performed using the optimal pumping policy, generated from the unconfined aquifer remediation problem using the embedded confined transition equation.

The optimal locations of the pumping well generated by the embedded, confined, and unconfined transition equation differ markedly (Table 6). The penalties are small for the two optimal designs but large for the comparative simulation (Table 7). The large penalty implies

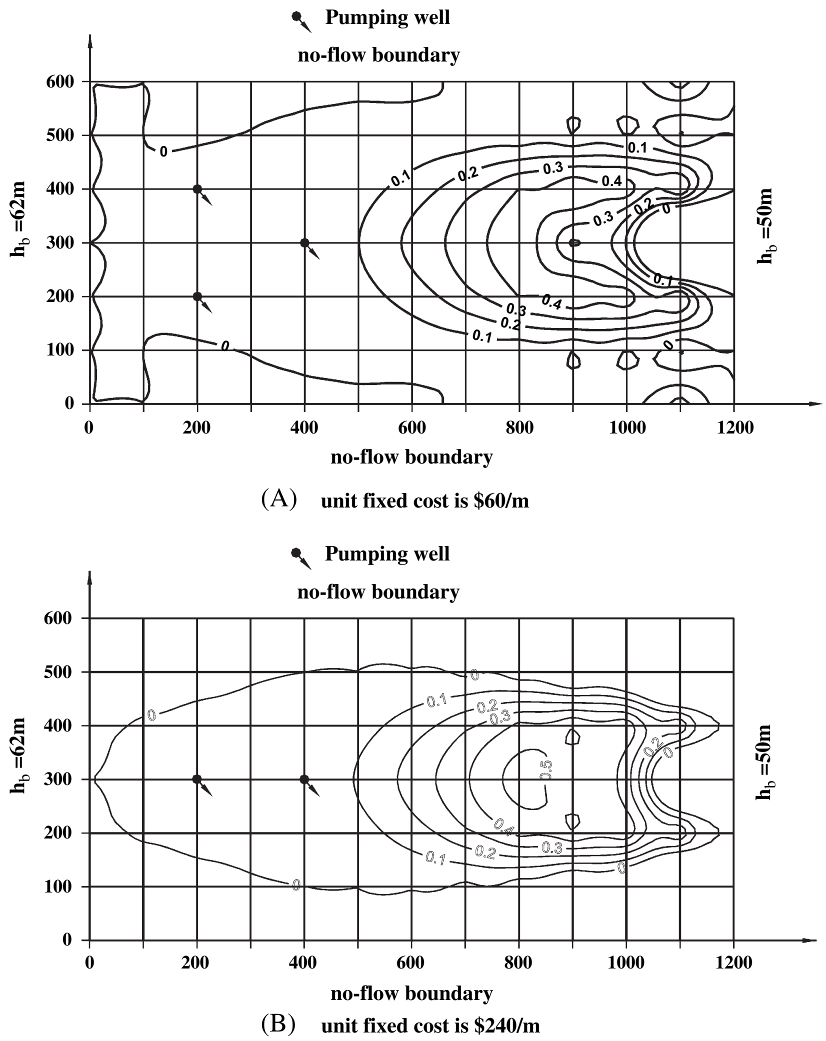


**Figure 3. Optimal network design and pollutant concentration distribution at the end of the planning period, for cases with unit fixed costs of \$60 and \$240/m.**

**Table 6**
**Optimal Pumping Sites Obtained by the Planning Model with an Embedded, Confined, or Unconfined Transition Equation**

| Unit Fixed Cost | $0/m | $60/m | $240/m |
|---|---|---|---|
| Confined | 17, 19, 24, 26, 31, 32, 33, 38, 40, 45, 47, 59, 61 | 24, 26, 32 | 18, 39 |
| Unconfined | 17, 19, 24, 26, 31, 32, 33, 38, 40 | 17, 19, 32 | 18, 32 |

The node number can be found in Figure 1.

that the optimal design obtained by the management model with the embedded confined transition equation fails to meet the required concentration constraints when the optimal design is reevaluated using an unconfined model. A plot of the time-varying concentration at node 66 in the three cases with a unit fixed cost of $60/m (Figure 4) indicates that the concentration of contaminants at the end of the planning period determined by the comparative simulation, simulated by the unconfined model and the pumping policy obtained from the management model with the embedded confined simulator, is ~1.0 ppm, which exceeds the required concentration of 0.5 ppm. Hence, the optimal design obtained using the management model with the embedded confined transition equation is not a feasible solution for an unconfined aquifer. Therefore, the management model of an unconfined aquifer requires an unconfined simulator, especially for small remediation sites, which exhibit largely varying hydraulic heads.

## Examples with Aquifer Heterogeneity

These examples illustrate the capacity of the proposed algorithm to solve a remediation design problem with aquifer heterogeneity and examine its effect on the optimal design. In the preceding cases, the unit fixed cost ($a_1$) and the hydraulic conductivity were assumed to be constant. However, this assumption is unlikely because aquifers are generally heterogeneous. In such cases, the unit fixed cost $a_1$ and hydraulic conductivity are spatially varied to simulate geological heterogeneity. A series of numerical examples illustrate the geological effects. The study area is separated into two subareas with different unit fixed costs and hydraulic conductivities (Figures 5 and 6). For uniform geological conditions and a constant fixed cost (Figure 3), the algorithm tends to select pumping wells from subarea I in which the initial concentration and hydraulic head are higher. Figure 5A demonstrates that all pumping wells are located in subarea I in which the hydraulic conductivity is lower than in subarea II. However, optimal pumping wells are located in subarea II (Figure 5B), after the spatial distribution of the hydraulic conductivity has been swapped.

Most wells are located in zone I because a well therein is cheaper than in zone II (Figure 6A). However, the pumping wells are concentrated in zone II, where well installation is cheaper (Figure 6B). The number and locations of wells also vary according to the magnitude and distribution of fixed costs, which depend on the geological conditions. Figures 5 and 6 cannot easily be derived for a conventional network design procedure that neglects fixed cost. Therefore, the proposed GCDDP algorithm provides a design that is nearer to the true optimal solution than that provided by conventional algorithms.

## Other Computational Issues

Efforts to implement particular programming techniques to increase computational efficiency are an expected response to the complexity of the proposed remediation problem. Four approaches, two of which have been implemented here, can accelerate the computation. The first increases the computational efficiency of the CDDP algorithm. Accelerating the CDDP algorithm reduces the computational time of the GCDDP algorithm since each chromosome in the GCDDP algorithm requires a CDDP computation. The computing time for CDDP is reduced herein by exploring the sparse structure of the state derivative matrices of the transition function ($\partial T/\partial x_t$)

**Table 7**
**Cost Comparison for Confined and Unconfined Transition Equation Models**

| | Unit Fixed Cost = $0/m | | Unit Fixed Cost = $60/m | | Unit Fixed Cost = $240/m | |
|---|---|---|---|---|---|---|
| | OC | Penalty | OC | Penalty | OC | Penalty |
| Confined | 154.2 | 0.000169 | 154.9 | 0.000160 | 186.9 | 0.000265 |
| Unconfined | 183.1 | 0.000059 | 187.1 | 0.000155 | 203.7 | 0.000010 |
| Simulation | 153.1 | 2352.1 | 153.8 | 1739.9 | 185.6 | 901.9 |

OC = operation cost. The value of operation cost and penalty is divided by 1000. Simulation denotes the unconfined aquifer model simulating the optimal policy, given from the unconfined aquifer remediation problem using the embedded confined transition equation.

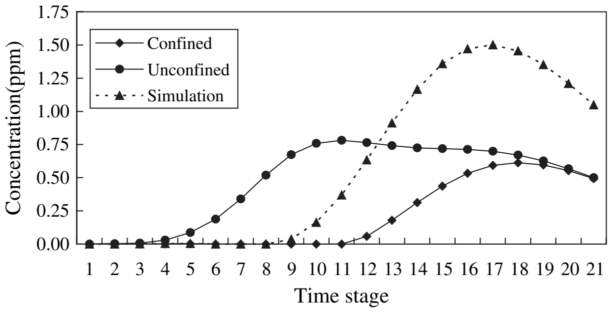


**Figure 4. Time-variant concentration at node 66 for a unit fixed cost of $60/m.**

(Mansfield et al. 1998). The CPU times for the algorithm that considers sparseness are ~5% lower than that for those that do not (Table 8).

The second method is bookkeeping. This method reduces the number of chromosomes to be evaluated by the CDDP algorithm. As mentioned previously, a network design (a chromosome) is a subset of all candidate sites. In the GA computation, a very fit chromosome is more likely to survive than an unfit one. Moreover, the number of the subsets (the chromosome) is countable and finite because the number of candidate sites is limited. Therefore, this investigation indicates that a very fit chromosome is likely to repeat itself from generation to generation in the GA computation. Hence, a bookkeeping procedure is performed to record all evaluations of chromosomes by the CDDP algorithm. A new chromosome is compared to a previously recorded one in each generation of the GCDDP algorithm. A CDDP computation is not required if the chromosome already exists, and the algorithm proceeds to the next chromosome. The case with unit fixed costs of $240/m illustrates the efficiency of the method. Notably, convergence requires 16 generations. The total number of required chromosomes is 1050; however, the CDDP algorithm calculates only 178 distinct chromosomes. Therefore, the bookkeeping method eliminates the calculation of ~83% of the chromosomes by the CDDP algorithm. The number of calculated chromosomes falls rapidly and saves significant CPU resources (Figure 7). The encoding of the chromosome is efficient because each well requires only a single bit and the additional memory required to implement the bookkeeping is minor.

Parallel computation is the third method for increasing computational capability. The GA is known to exhibit simple and highly efficient parallelism, confirming its

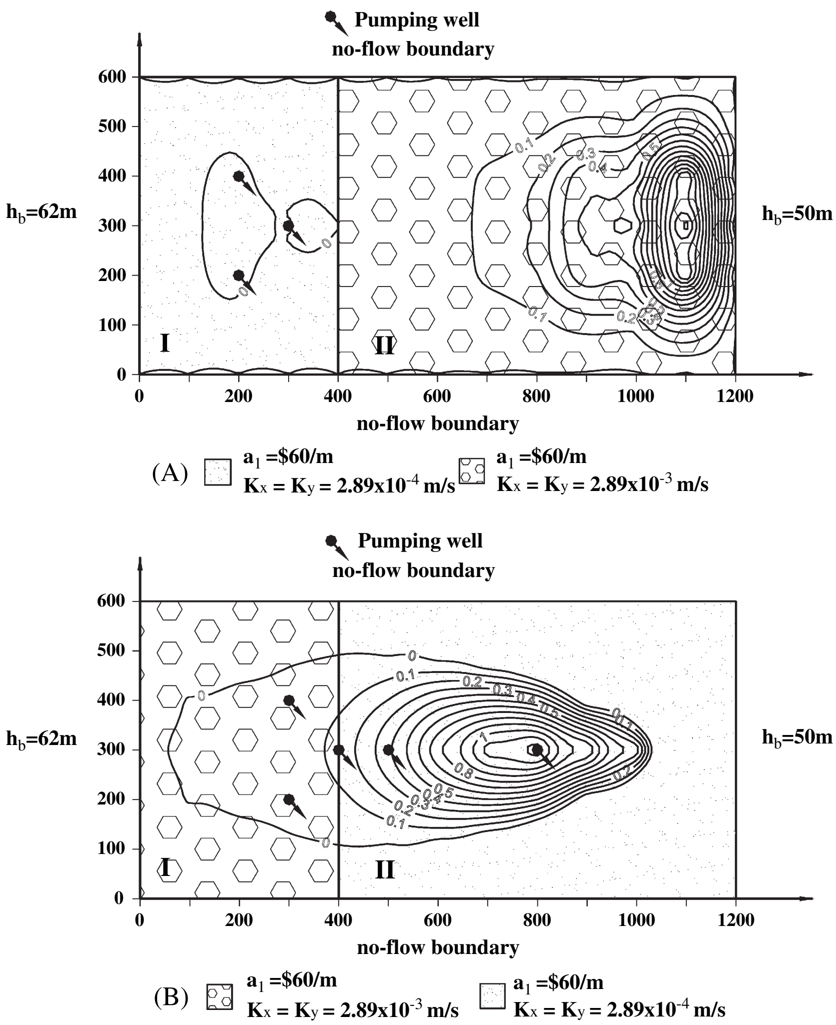


**Figure 5. Optimal number of wells and concentration distribution for geological heterogeneity with a unit fixed cost of $60/m.**

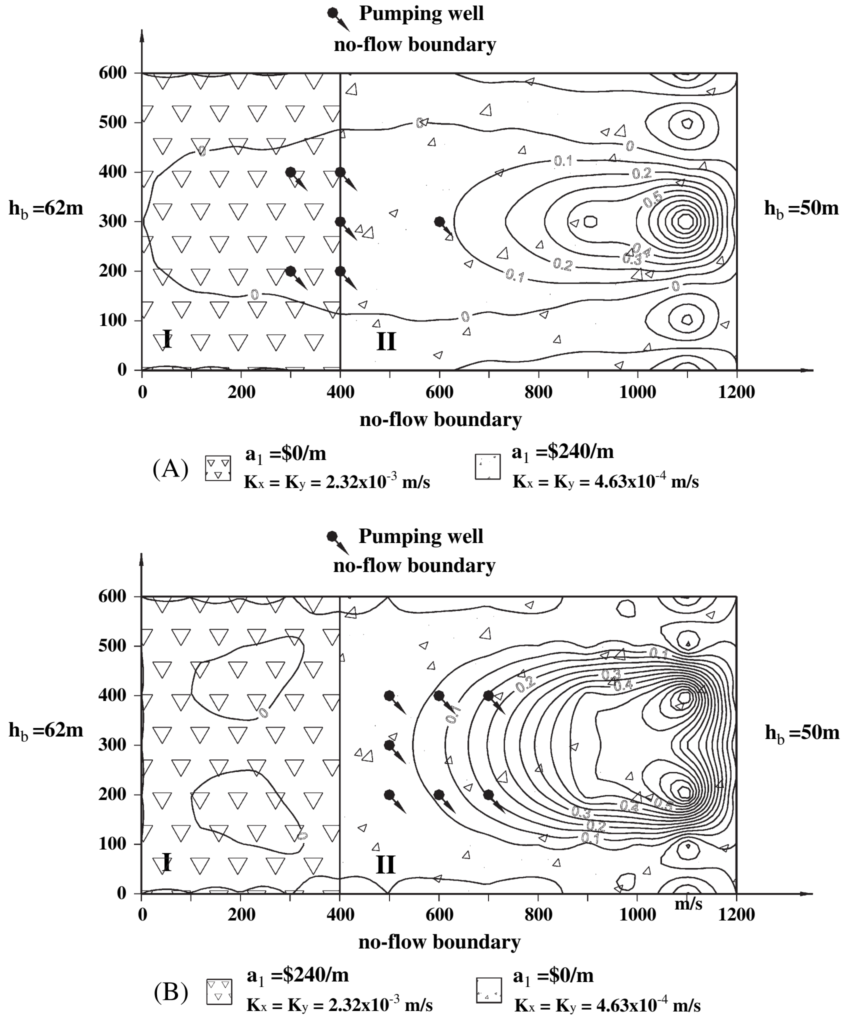


**Figure 6. Optimal number of wells and concentration distribution for unit fixed costs varying with geology.**

superiority over other combinatory algorithms such as simulation annealing and tabu search, in solving a ground water remediation design problem. This study does not review parallel computing, but the proposed model can be constructed in parallel. In the GCDDP algorithm, ~98% of CPU time is spent on evaluating chromosomes (CDDP computing), which would benefit from parallel computing, since each chromosome is determined independently. Therefore, parallel computing can significantly increase the computational capacity of the GCDDP algorithm and solve large-scale problems.

In addition to the three strategies mentioned for improving computational efficiency of a heuristic search method, the response function (or surrogate model) is another important one. With this approach, a response function between the objective function and decision variables is established after a sufficient number of simulation runs. The response function may then serve as a surrogate model in lieu of the numerical simulation model, significantly reducing the computation run times (Zheng and Wang 2002).

**Table 8**
**CPU Time per Iteration with/without Employing the Sparsity in CDDP Algorithm for Unconfined Aquifer Remediation**

| | CPU Time per Iteration (s) | | |
|---|---|---|---|
| **Coefficient $a_1$** | **$0/m (seven wells)** | **$60.0/m (three wells)** | **$240/m (two wells)** |
| With employing the sparsity ($T_1$) | 3.00 | 2.90 | 2.86 |
| Without employing the sparsity ($T_2$) | 3.14 | 3.06 | 3.00 |
| Ratio of difference (($T_2 - T_1$)/$T_2$) (%) | 4.46 | 5.23 | 4.67 |

Runs are performed on a PC with an AMD Athlon™ 1000-MHz CPU.

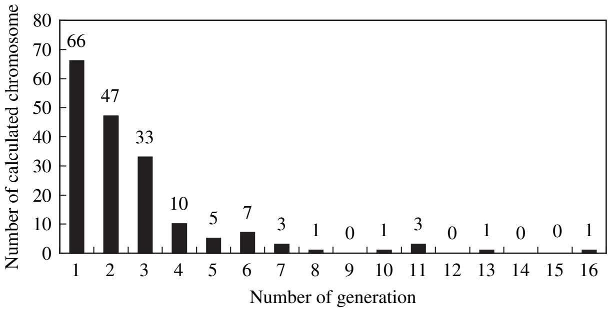


**Figure 7. Calculated chromosome through 16 generations for unit fixed cost of $240/m.**

## Conclusion

An unconfined aquifer remediation model, GCDDP, was presented to minimize the total cost of remediation under pump and treat, considering both fixed costs and time-varying operating costs. The model integrates GA and CDDP. The total cost, including the fixed and operating costs, is the objective function of a ground water remediation problem. This total cost had not been previously addressed because of the combinatory and dynamic characteristics of the problem. This investigation calculated the fixed cost term using GA and evaluated the time-varying operating costs using the CDDP algorithm.

When the optimization model neglects fixed costs, the GCDDP algorithm consistently designs a remediation plan with numerous wells pumping at low rates. However, incorporating the fixed costs can reduce the number of wells and affect their locations in the network design. Hence, the GCDDP design can provide significant savings by considering the fixed costs. Using the confined model instead of the unconfined model can avoid the need to solve the nonlinear flow equation and the derivative calculations of the unconfined aquifer. However, this approximation can cause the solution obtained by the confined model to fail to satisfy the required water quality standard, when the design is reviewed by an unconfined model. The test cases demonstrate that when the flow domain is heterogeneous, the number and locations of pumping wells may vary with the fixed cost, determined by hydrogeological conditions. This phenomenon cannot easily be determined using a conventional network design procedure that neglects fixed cost. This investigation improves the computational efficiency of the proposed GCDDP algorithm at the expense of an increase in the computational burden by considering the sparse structure of the state derivative matrices of the transition equation and applying a bookkeeping programming procedure. The GCDDP algorithm is thus a feasible ground water remediation planning approach. In summary, the novel GCDDP algorithm considers fixed cost, which is important in ground water remediation planning, to provide a more realistic solution. Parallel computation can further improve the computational capacity of GCDDP to solve large-scale problems and is currently being investigated.

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