Optimal control algorithm and neural network for dynamic groundwater management

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Abstract:

Researchers have found that obtaining optimal solutions for groundwater resource-planning problems, while simultaneously considering time-varying pumping rates, is a challenging task. This study integrates an artificial neural network (ANN) and constrained differential dynamic programming (CDDP) as simulation-optimization model, called ANN-CDDP. Optimal solutions for a groundwater resource-planning problem are determined while simultaneously considering time-varying pumping rates. A trained ANN is used as the transition function to predict ground water table under variable pumping conditions. The results show that the ANN-CDDP reduces computational time by as much as 94·5% when compared to the time required by the conventional model. The proposed optimization model saves a considerable amount of computational time for solving large-scale problems. Copyright © 2009 John Wiley & Sons, Ltd.

KEY WORDS   neural network; constrained differential dynamic programming (CDDP); groundwater management

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INTRODUCTION

Groundwater is a valuable water resource with many diverse uses for domestic, agricultural, and industrial purposes. Previous studies have extensively explored ways to ensure sustainable ground water use, owing to its importance. Research has employed many optimization techniques in groundwater management planning, including linear programming, nonlinear programming (Gorelick *et al.*, 1984; Ahlfeld *et al.*, 1988), mixed-integer programming (Rosenwald and Green, 1974), genetic algorithms (GA) (McKinney and Lin, 1994; Wang and Zheng, 1998), and constrained differential dynamic programming (CDDP). Temporal water-resource systems require that any simulation or optimization model be dynamic in order to yield satisfactory results, unless the input assumptions justify a static system. For groundwater supply, the demand for groundwater may vary over time, particularly when the aquifer operates conjunctively with the surface water system (Basagaoglu *et al.*, 1999). Among these methods, CDDP exploits the sequential time structure of these problems (Jones *et al.*, 1987). Using CDDP requires that dynamic optimal groundwater management accommodate these situations. CDDP significantly reduces dimensionality difficulties associated with nonlinear dynamic groundwater management problems (Jones *et al.*, 1987; Chang *et al.*, 1992; Culver and Shoemaker, 1992; Chang and Hsiao, 2002; Chang *et al.*, 2007). Jones *et al.* (1987) used CDDP algorithm for unsteady, nonlinear, groundwater management problems. Due to the stage-wise decomposition of CDDP, the dimensionality problems associated with embedding the hydraulic equations as constraints in the management model are significantly reduced. 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 contaminated aquifer remediation. Culver and Shoemaker (1992) found that time-varying policies are more cost-effective than time-invariant policies. The CDDP used herein is a modification of SALQR and has been shown efficient in solving time-varying problems. However, computational burdens that accompany field-scale problems hinder using CDDP in actual projects (Mansfield *et al.*, 1998; Liu and Minsker, 2001).

Artificial neural network (ANN) consists of an interconnected group of neurons and processes information using a connectionist approach to computation (Coulibaly *et al.*, 2001; Pijanowski *et al.*, 2002). The ANN is an alternative modelling and simulation tool, especially for dynamic nonlinear systems (Coppola *et al.*, 2003a,b, 2005, 2007; Becker *et al.*, 2006; Feng *et al.*, 2008). Recently, many researchers have successfully applied ANN models in hydrologic modelling, such as typhoon rainfall forecasting (Lin and Chen, 2005), the determination of aquifer parameters (Samani *et al.*, 2007), and regional ground water levels simulation (Coppola *et al.*, 2003a,b, 2005; Feng *et al.*, 2008). A number of studies combine the optimization model with ANN (Rogers and Dowla, 1994; Rogers *et al.*, 1995; Johnson and Rogers, 2001; Rao *et al.*, 2003, 2005). Rogers and Dowla (1994) used ANN-GA methodology to replace

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the traditional simulation-optimization model. The model uses 20 pre-selected extraction locations with steady-state pumping rate to search for the subset producing the smallest volume of pumping water over a 40-year planning period. Rogers *et al.* (1995) also used ANN-GA methodology to locate the best pumping patterns for meeting remediation objectives. Rao *et al.* (2003) apply simulated annealing (SA) with an ANN, which replaces the SHARP (A numerical finite-difference model to simulate freshwater and saltwater flow separated by a sharp interface) interface flow model to meet demand during non-monsoon season without including excessive saltwater instruction. Rao *et al.* (2005) use ANN and SA for planning groundwater development in coastal deltas and a trained ANN as the SEAWAT (A computer program for simulation of three-dimensional variable-density groundwater flow and transport) model to predict final groundwater concentration under variable pumping condition. The above researches consider fixed pumping rate in the design problem, yet they lack system dynamic response, such as time-varying water level or concentration. Applying an optimization technique such as GA or SA to solve time-varying policies would dramatically increase computational resources required. Becker *et al.* (2006) indicated that simulation-optimization methods including the ANN-GA model are able to search better solutions than current trial-and-error approaches. The optimal objective function values are an average improvement of 20% than that of trial-and-error methods.

This study presents a novel approach for solving this optimization problem by effectively combining a CDDP with an ANN for groundwater management. The algorithm is a CDDP embedded with an ANN. The CDDP computes the optimal time-varying pumping schemes to minimize the operating cost present value while meeting water demand constraints. The embedded ANN computes the system response and hydraulic head, for a pumping policy.

FORMULATION OF THE PROPOSED MANAGEMENT MODEL

The management model contains an aquifer, which is a two-dimensional unconfined system. The governing equation that describes groundwater movement is

$$\frac{\partial}{\partial x}\left(K_{xx}h\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_{yy}h\frac{\partial h}{\partial x}\right) + \sum_{i\in I}u_i\delta(x_i, y_i) = S_y\frac{\partial h}{\partial t} \quad (1)$$

where h denotes the hydraulic head, K_{xx} and K_{yy} represent the principal components of hydraulic conductivity aligned along x and y coordinate axes, I represents the set of pumping wells, S_y denotes the specific yield, u_i represents pumping rate located at (x_i, y_i), and $\delta(x_i, y_i)$ is the dirac delta function evaluated at (x_i, y_i). Equation (1) is subject to the appropriate initial and boundary conditions.

The management model is then formulated as follows:

$$\min_{u_t^i,\ i\in I, t=1,\dots,T} J = \sum_{i\in I}\{\sum_{t=1}^{T}c_2\,u_t^i[L_*^i - h_{t+1}^i]\frac{1}{(1+r)^t}\} \quad (2)$$

subject to

$$\{h_{t+1}\} = T(h_t, u_t, t),\ t = 1, 2, \dots, T \quad (3)$$

$$h_{t+1, j} \geq h_{\min},\ t = 1, 2, \dots, T,\ j \in \Phi \quad (4)$$

$$\sum_{i\in I}u_t^i \geq d_t,\ t = 1, 2, \dots, T,\ i \in I \quad (5)$$

$$u_{\min} \leq u_t^i \leq u_{\max},\ t = 1, 2, \dots, T,\ i \in I \quad (6)$$

where Equation (2) represents the operating cost present value associated with well network I. The decision variable is u_t^i which is pumping rate at pumping well i at time step t. The expression $L_*^i - h_{t+1}^i$ simply represents drawdown at pumping well i. $L_*^i(I)$ is the distance between the ground surface and the lower datum of the aquifer for each well; h_{t+1}^i denotes hydraulic head at pumping well i at time $t + 1$. The term r denotes the interest rate. The term c_2 denotes the cost coefficient of pumpage and is expressed as $c_2 = \gamma \times c_1 \times \Delta t$, with Δt as the duration of pumping, γ the specific gravity, and c_1 the unit cost of electric power. Equation (3), as derived from Equation (1), represents the system dynamics relation in the optimization. Equation (4) defines lower limits $h_{\min}$ on the hydraulic head to avoid damage caused by over-pumping. Equation (5) represents the requirement that total demand d_t for groundwater supply must be satisfied. The upper limits of Equation (6) denote the capacity of each well while the lower limits can be applied to avoid well installation that has small pumping rates, which are obviously infeasible. $u_{\min}$ and $u_{\max}$ denote the minimum and maximum pumping rate for each well. I is an index set defining a pumping network and the upper index i denotes a well in the network design I; Φ represents the set of observation wells.

INTEGRATION OF CDDP AND ANN

This study integrates CDDP and ANN to develop the groundwater management model that is CDDP with ANN embedded in the optimal present operating cost evaluation for time-varying pumping defined by Equations (2) to (6). Figure 1 shows the procedure to develop the ANN-CDDP model. The approach confronts the problem by training ANN to predict system response. Although ANN is trained, the ANN can be coupled with CDDP. The CDDP can be used to evaluate optimal operating costs present value. The details are further explained as follows:

Step 1: Create training data by repeated case simulation using ISOQUAD

The current work generates training data from 3000 simulation data by an aquifer simulation model (ISOQUAD
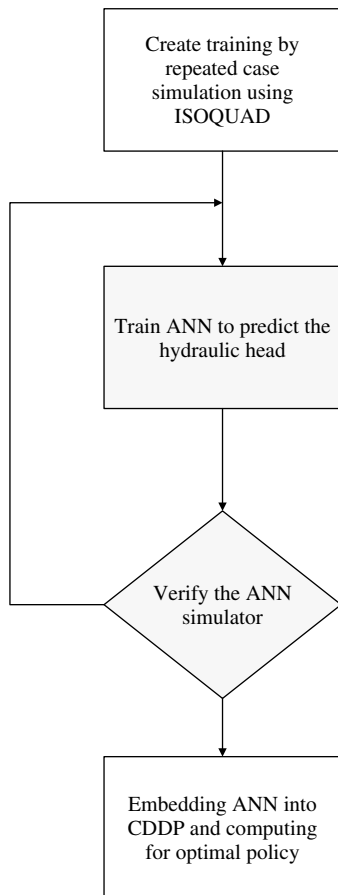
$$O_j = f(net_j), \ net_j = \sum_i w_{i,j}O_i - b_j \qquad (7)$$

where O_j denotes the output for node j in the output layer; O_i denotes the input for node i in the input layer; f is transfer function; $w_{i,j}$ denotes a connected weight between jth node in the output layer with ith node in the input layer; b_j represents bias value in the output layer.

This paper uses the ANN as a dynamic simulator for determining hydraulic head at time $t + 1$, which is based on the pumping rate and hydraulic head at time t. The ANN training can be done by providing it with dynamic behaviour information as shown in Figure 2. Equation (8) is written as the input-output pattern of ANN, where the output, which is the hydraulic head (h_{t+1}) at time $t + 1$ is a function of inputs including the pumping rate (u_t) and hydraulic head (h_t) at time t:

$$h_{t+1} = f(h_t, u_t), \ t = 1, 2, \ldots, T \qquad (8)$$

The dimension of input vector in Equation (8) is $m + n$ and the output state vector is n, where n is the number of observation wells and m is the number of pumping wells. For example, the ANN includes three inputs and two outputs if there are a pumping well and two observation wells.

Step 3: Embedding ANN into CDDP and computing the optimal policy

The CDDP is a successive approximation technique for solving optimal control problems and iteratively determining the optimal solution to the problem stated in Equations (2) to (6). Murray and Yakowitz (1979); Jones *et al.* (1987), and Chang *et al.* (1992) provide a detailed discussion of the CDDP algorithm. Compared with previous studies, Equation (3) is the transition function to simulate system response induced by control policy, and Equation (8) is the ANN model of ground water flow in this study.

The ANN-CDDP computes the optimal solution by resolving a series of quadratic problems, and the quadratic approximation of the original problem. The ANN-CDDP searches for the optimal policy and calculates optimal operating costs through the backward and forward sweep. In the backward sweep, the ANN-CDDP evaluates an update control policy through a series of

Figure 1. Flow chart for ANN-CDDP

(Pinder, 1978)). The total available data has been divided into two sets, training and validation set: approximately 2500 patterns (samples) were used to train the ANN, and 500 different patterns were used for validation. Here, the unconfined aquifer simulator is modified from the ISOQUAD (Pinder, 1978), a two-dimensional confined aquifer simulator, using the Picard method (Hsiao and Chang, 2005). The ISOQUAD is the numerical solution obtained by applying the Galerkin finite-element method for the space derivative and an implicit finite difference scheme for the time derivative.

Step 2: Train ANN to predict hydraulic head

The ANN attempts brain simulation (Biological neural network). The architecture used for ANN is a feed-forward network, trained by the back-propagation learning algorithm (Tsai and Lee, 1999; MATLAB, 2000; Rao *et al.*, 2003, 2005; Coppola, 2003a). ANN has the phases of neural processing: learning is the process by which ANN data is encoded with weights. After learning completion, the weights and bias are updated from the learning process. The recall process retrieves information based on weights obtained from the learning process and predicts output data of a new example. The functions for a two-layer neural network can be written as (Negnevitsky, 2002; Coppola *et al.*, 2003a; Kumar, 2004; Samani
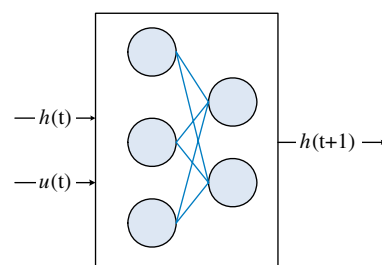

Figure 2. ANN architecture for the study

matrix computations with derivative information. The derivatives in the transition equation, $\frac{\partial O_j}{\partial O_i}$, are derived by a single-layer ANN in the following.

$$\frac{\partial O_j}{\partial O_i} = w_{i,j} \cdot \frac{\partial f(net_j)}{\partial net_j} \qquad (9)$$

For a multi-layered network, the derivatives in the transition equation are derived by ANN in the following (Dimopoulos *et al.*, 1995; Yang and Chang, 2001):

$$\frac{\partial O_k}{\partial O_i} = \sum_{jn} \sum_{jn-1} \sum_{jn-2} \cdots \sum_{j1} w_{jn,k} \frac{\partial f(net_k)}{\partial net_k}$$
$$\cdot w_{jn-1,jn} \cdot \frac{\partial f(net_{jn})}{\partial net_{jn}} \cdot w_{jn-2,jn-1}$$
$$\cdot \frac{\partial f(net_{jn-1})}{\partial net_{jn-1}} \cdots w_{i,j1} \cdot \frac{\partial f(net_{j1})}{\partial net_{j1}} \qquad (10)$$

where O_k denotes the output for node k in the output layer; jn, $jn-1, \ldots,$ and $j1$ denote the neural units in the nth, $n-1$th,..., and 1st hidden layer.

While ANN-CDDP is in the forward sweep, ANN can specify the value of state variables at each time step, using the initial value of state variables and the transition equation, Equation (3). Reapplying quadratic programming solves the problem and reveals optimal policy. The computed optimal policy becomes the nominal policy for the next iteration. Unless this step satisfies the stopping criterion, iterations are required.

RESULTS AND DISCUSSION

This study adopts a ground water supply problem, which is a modification of the example from Hsiao and Chang (2002) to verify the methodology effectiveness. Figure 3
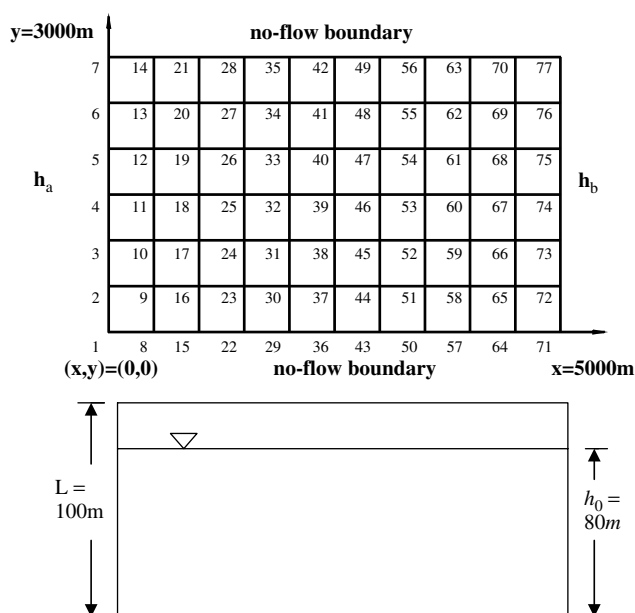
Table I. Aquifer properties and simulation parameters of cases

Parameter	Value
Aquifer thickness	100 (m)
Initial ground water head	80 (m)
Horizontal hydraulic conductivity	0·005 m/s
Vertical hydraulic conductivity	0·005 m/s
Porosity	0·2
Specific yield	0·1
Cost per kilowatt-hour	$1·35

displays a hypothetical and unconfined aquifer to demonstrate the algorithm performance described above. The 3000 m × 5000 m site includes 77 finite-element nodes, 60 elements, and 5 pumping well locations. No-flow and constant-head boundaries ($h_a = h_b = 80$ m) circumvent the flow domain. This work assumes that initial conditions on hydraulic head distribution prior to pumping are steady state. Aquifer properties and simulation parameters are listed in Table I. The initial conditions on hydraulic head are $h_0 = 80$ m and the distance between the aquifer bottom and ground surface is $L = 100$ m. This study calculates the present value of the optimal operating cost of a well system, which satisfies the maximum demand of each time step. The following three cases discuss the effects of water demand curve, total demand, and model size for the numerical experiment.
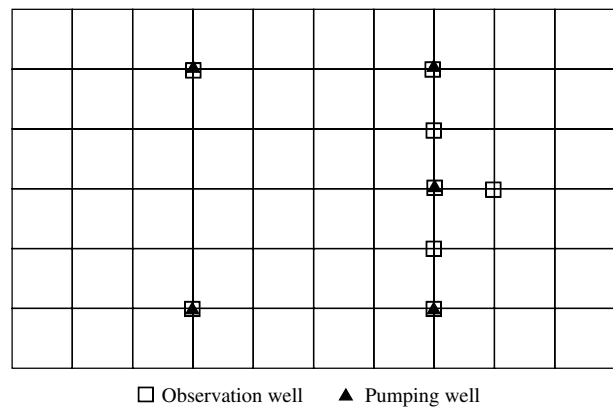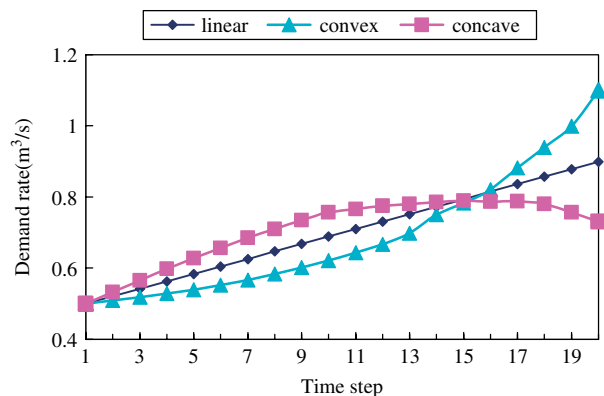

Figure 4. Plan view of Case 1 and Case 2

Figure 3. The aquifer for water supply in Cases 1 and 2

Figure 5. Water demand increasing curves in Case1

Case 1: Comparing varying water demands over a period of 5 years

Figure 4 shows Case 1 and 2, including five pumping wells (black triangle) and eight observation wells (open square). This section compares the operation costs of the pumping policy under each of the three water demand curves (i.e. linear, concave, and convex) (Basagaoglu and Yazicigil, 1994), as illustrated in Figure 5. The total water demand over 5 years is assumed as 110 ($10^6 m^3$). The management model for Cases 1 and 2 divides the planning horizon into 20 stages over 5 years and each time step (Δt) is 91·25 days.

There is a three-layer feed-forward network in the study. Two thirds of the input neuron number is defined as the hidden neuron number; this can generate results of almost similar accuracy but requires much less time to train (Wang, 1994). In this model, ten hidden neurons are used in the network to ensure a balance of both accuracy and computation effort. The ANN inputs are the pumping rate and hydraulic head at current time and the outputs are hydraulic head at future time. The inputs dimension is the 13 and outputs dimension is the 8 where the pumping well numbers are 5 and the observation well numbers are 8. The transfer functions in the model are hyperbolic tangent sigmoid for hidden layers and linear for the output layer. The neural network model is trained using an ANN toolbox by MATLAB (2000). A network training function updates weight and bias values according to Levenberg-Marquardt optimization. The stopping criterion is based on the mean squared error (MSE) = 10^{-5}. If the stopping criteria are not met, the algorithm will continue. After ANN training, this experiment quantifies error with ANN and the ISOQUAD solution, using the root mean squared error (RMSE). For the validation data sets, the RMSE of Case 1 is 0·004 m in average. The relative validation error with respect to average ground water level is small, illustrating high predictive performance. The ANN predicts hydraulic heads accurately at the selected control locations under variable pumping conditions but condensed surrogate for ground water flow model in the representative nodes (Coppola *et al.*, 2003a,b; Feng *et al.*, 2008). The operating cost present value of the optimal policy is illustrated in Table II. The operating cost present value is most expensive for the concave curve and least expensive for the convex curve. Accuracy of the proposed model can be quantified by comparing it with the ISOQUAD-CDDP (Chang *et al.*, 1992; Culver and Shoemaker, 1992). Results demonstrate that relative error is 0·03% or less when calculating costs.

Case 1·1, with convex water demand, has the least operating cost present value. Case 1·2, with linear water demand, has the middle present value of operating cost. Case 1·3, with concave water demand, has the most operating cost present value. This study explains why the operational cost for a concave case is more than that for linear and convex cases. Comparing the convex curve with the linear and convex curve indicates that the convex curve (Case 1·1) needs less water at early stages than the other two curves, and has relatively more requirements at the late stage. Figure 6 shows the optimal pumping rates determined by ANN-CDDP and ISOQUAD-CDDP in Case 1. The optimal pumping rates obtained from the two models are approximate, indicating that the ANN-CDDP model is a feasible alternative of ground water management. The figures also imply a relationship between time-varying pumping rate and demand under different curves. Case 1·1 has more water pumping than the other cases near the end of the planning period since the pumping rate is related to water demand (Figure 6). Based on economic theory, investing $1 today will yield more than investing $1 tomorrow (Chang *et al.*, in press). Nevertheless, computing present operation cost value near the ending time has more discounting effect. Case 1·1 has the least operating cost present value. The illustrations explain the resulting optimal operational cost of three cases.

Case 2: Comparison of total water demand influence on cost over a period of 5 years

When the total convex water demand curve increases from 110 ($10^6 m^3$) to 160 ($10^6 m^3$), the optimal management model satisfies the different water demands. The experiment embeds CDDP with ANN, which the ANN determines future hydraulic head based on the current pumping rate and hydraulic head. The ANN is same to Case 1 on the same boundary, time interval, and well locations. Figure 7 shows the optimal pumping rates determined by ANN-CDDP in Case 2. Results in the figure imply a relationship between time-varying pumping rate and demand: the pumping rate increases when water demand increases. Results are consistent with the Equation (1) that indicates the more the pumping volume, the higher the operation cost. Therefore, the operation cost trend in time is relative to their demand curves (Chang, *et al.*, in press).

This study finds that optimal pumping strategies satisfy these total demands using ANN-CDDP and ISOQUAD-CDDP. Table III shows that operation cost increases when water demand increases and the accuracy of ANN-CDDP used can be quantified when compared with

Table II. Comparison of ANN-CDDP and ISOQUAD-CDDP solutions in case 1

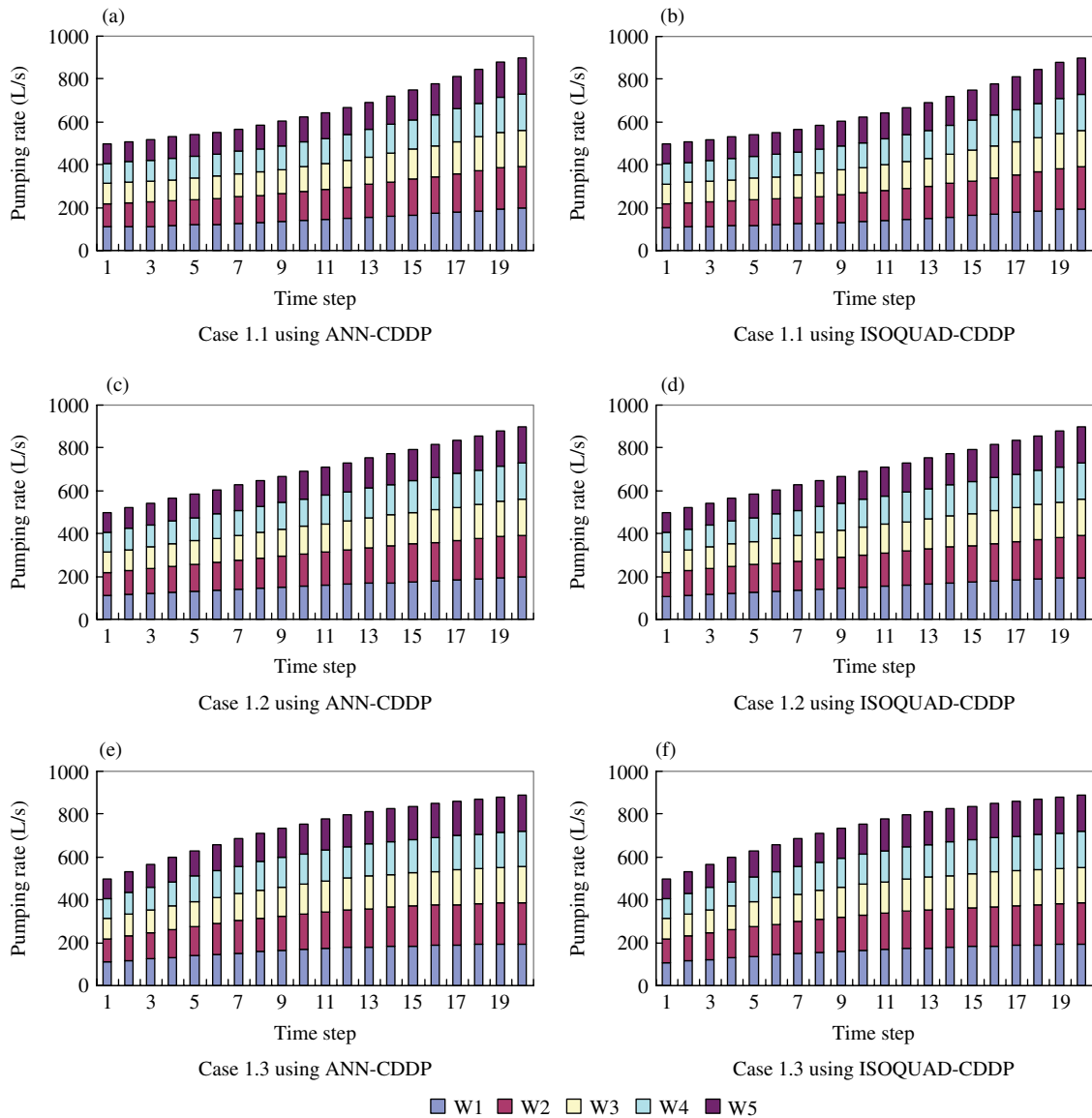|	Water demand curve form	Optimal operating cost using ANN-CDDP ($)	Optimal operating cost using ISOQUAD-CDDP ($)	Relative error (%)
Case 1.1	Convex	125 027	125 035	0·01
Case 1.2	Linear	133 514	133 539	0·02
Case 1.3	Concave	142 041	142 089	0·03

Figure 6. Total pumping rates at each period in Case 1 using ANN-CDDP and ISOQUAD-CDDP
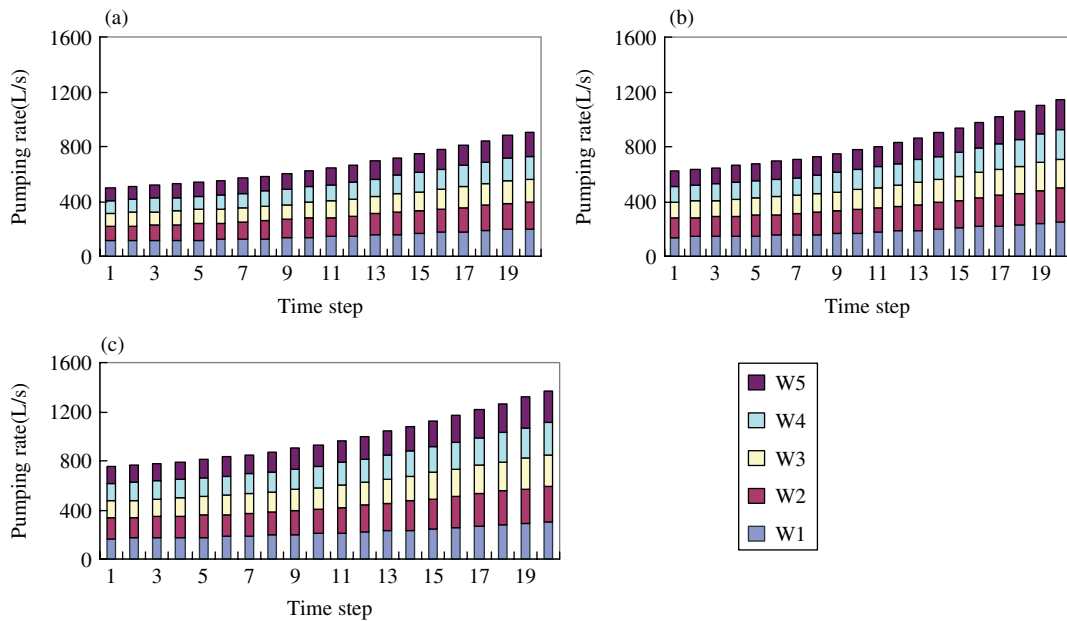

Figure 7. Total pumping rates at each period using ANN-CDDP in (a) Case 2·1, (b) Case 2·2, and (c) Case 2·3

Table III. Comparison of ANN-CDDP and ISOQUAD-CDDP solutions in case 2

	Demand	Optimal operating cost using ANN-CDDP ($)	Optimal operating cost using ISOQUAD-CDDP ($)	Relative error (%)
Case 2·1	110 ($10^6 m^3$)	133 514	133 539	0·02
Case 2·2	135 ($10^6 m^3$)	164 932	164 962	0·02
Case 2·3	160 ($10^6 m^3$)	197 213	197 270	0·03

Table IV. Three case sizes in case 3

	Number of nodes	Number of elements
Case 3·1	91	72
Case 3·2	187	160
Case 3·3	315	280

□ Observation well ▲ Pumping well
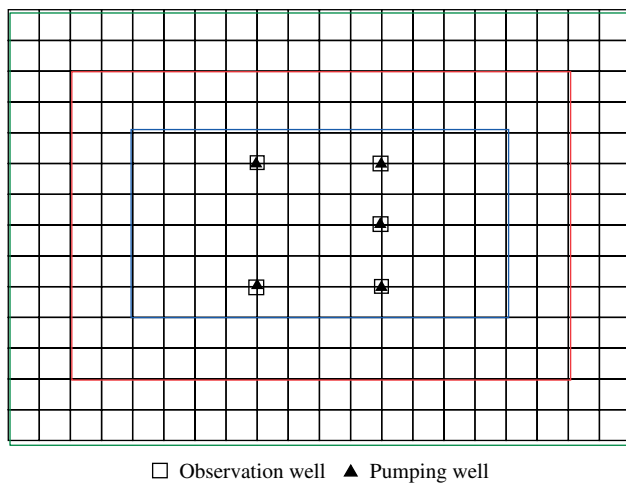
Figure 8. Plan view of Cases 3·1 (blue), 3·2 (red), and 3·3 (green)

the number of finite-element nodes and elements in the three cases. Figure 8 indicates the three different domains with finite-element mesh, along with five pumping wells (black triangle) and five observation wells (open square). The boundary conditions, initial conditions, and aquifer properties are the same for Case 1. Table I lists the aquifer properties and simulation parameters. Based on the 5-year water demand schedule, the planning horizon is divided into 60 time steps and each time step in the management model (Δt) is 30·4 days. Total amount of water demand is 125 ($10^6 m^3$) for each case and the water demand curve is assumed linear.

The ANN training data are generated independently from the simulation results based on different domain sizes. ANN models are trained using the above-described procedures, and the input dimension is 10 and the output dimension is 5 where the pumping well numbers are 5 and observation well numbers are 5. After training and validation, ANN is embedded in CDDP and the current study compares the present operating cost value under different domain sizes between ANN-CDDP and ISOQUAD-CDDP. Results show that the difference in cost between ISOQUAD-CDDP and ANN-CDDP for

ISOQUAD-CDDP: the results demonstrate that relative error of cost is less than 0·05%. Findings show that increasing demand has no significant effect on the proposed model accuracy. ANN-CDDP has the ability to minimize the operating cost under the variant total water demands. Thus, ANN-CDDP is an alternative way for the dynamic ground water supply optimization.

Case 3: Comparison of the influence of different domain sizes

This study presents the solutions obtained for three hypothetical, isotropic, unconfined aquifers with different dimensions: 600 m × 1200 m (blue), 1000 m × 1600 m (red), and 1400 m × 2000 m (green). Table IV indicates
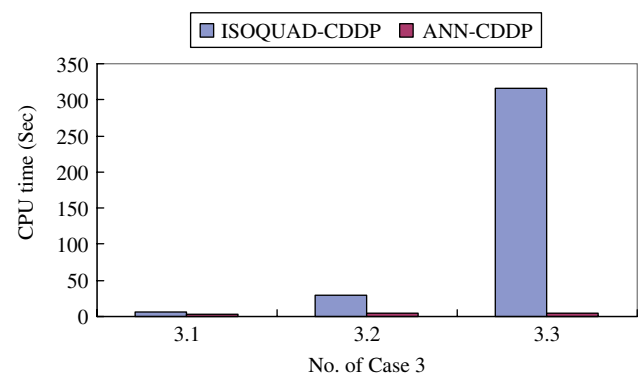

Figure 9. Comparison of CPU time each iteration between ANN-CDDP and ISOQUAD-CDDP at Case 3

Table V. Comparison of ANN-CDDP and ISOQUAD-CDDP solution and CPU time (maximum iteration number is fifty) in case 3

		ANN-CDDP	ISOQUAD-CDDP	Relative error (%)
Case 3·1	Optimal operating cost ($)	154 892	154 863	0·02
	CPU time each iteration (s)	3·79	5·74	
Case 3·2	Optimal operating cost ($)	156 033	156 022	0·01
	CPU time each iteration (s)	4·37	29·33	
Case 3·3	Optimal operating cost ($)	157 278	157 268	0·01
	CPU time each iteration (s)	4·30	316·26	

each case is 0·02% or less. Comparing central processing unit (CPU) iteration time (maximum iteration number is 50) with both methods, findings in Table V and Figure 9 show that computational work for ANN-CDDP in this study does not increase with domain size. The findings also provide support for the hypothesis that computational work for the ISOQUAD-CDDP model is proportional to O (Ns^3), where Ns is the total number of state variables (Mansfield *et al.*, 1998; Liu and Minsker, 2001). Thus, computational work between both is proportional to domain size. Case 3·3 presents a comparative table involving ISOQUAD-CDDP and ANN-CDDP from which show that the latter saves significant computational time. The ANN-CDDP reduces computational time by as much as 94·5% compared to the time required by the ISOQUAD-CDDP.

CONCLUSIONS

In optimization model, the number of state variables might be considerable and lead to a computational burden with real world problems. Therefore, this paper proposes a new optimization approach in dynamic groundwater management. The proposed model, which integrates a neural network (ANN) and CDDP, calculates the optimal operation cost by considering time-varying pumping rates for ground water resources management. The proposed methodology can handle large-field problems by using the number of observed states irrespective of domain size. The ANN-CDDP reduces computational time by as much as 94·5% compared to the time required by the conventional model (ISOQUAD-CDDP). The problem is less complex using this methodology than the conventional model. Results show that the methodology is suitable for the large-field control purposes.

Sub-surface pollutant transport is a dynamic process. Solving large field-scale problems related to groundwater remediation design is time-consuming, as the search may require numerous simulation runs for optimal remediation strategies. The ANN program extends to simulate time-dependent behaviour in coupled flow and solute-transport. This study therefore proposes using the ANN-CDDP model to solve remediation design problems in the future.

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