Water Resour Manage (2012) 26:1253–1269
DOI 10.1007/s11269-011-9957-0

Integration of Optimal Dynamic Control and Neural Network for Groundwater Quality Management

Liang-Cheng Chang · Hone-Jay Chu · Chin-Tsai Hsiao

Received: 15 May 2010 / Accepted: 6 December 2011 /
Published online: 20 December 2011

Abstract This study integrates an artificial neural network (ANN) and constrained differential dynamic programming (CDDP) to search for optimal solutions to a nonlinear time-varying groundwater remediation-planning problem. The proposed model (ANN-CDDP) determines optimal dynamic pumping schemes to minimize operating costs and meet water quality requirements. The model uses two embedded ANNs, including groundwater flow and contaminant transport models, as transition functions to predict groundwater levels and contaminant concentrations under time-varying pumping. Results demonstrate that ANN-CDDP is a simplified management model that requires considerably less computation time to solve a fine mesh problem. For example, the ANN-CDDP computing time for a case involving 364 nodes is 1/26.5 that of the conventional optimization model.

Keywords Neural network · Constrained differential dynamic programming · Groundwater quality · Optimization

1 Introduction

Ground water is a valuable water resource available on earth with diverse uses for domestic, agricultural, and industrial purposes (Philbrick and Kitanidis 1998; Basagaoglu and Marino 1999; Feuillette et al. 2003; Chang et al. 2007; Chu and Chang 2009a; Chu and Chang 2010). However, groundwater contamination occurs when man-made products such as gasoline, oil,

L.-C. Chang
Department of Civil Engineering, National Chiao Tung University, 1001 TA Hsueh Road, Hsinchu, Taiwan 300

H.-J. Chu (✉)
Department of Geomatics, National Cheng Kung University, No.1, University Road, Tainan City 701, Taiwan
e-mail: honejaychu@gmail.com

C.-T. Hsiao
Department of Information Management, Chung Chou University of Science and Technology, No. 6, Lane 2, Sec. 3, Shanjao Rd., Yuanlin Township, Changhua County 510, Taiwan
e-mail: cthsiao.hsiao@gmail.com

waste disposal practices and chemicals mix with groundwater. To ensure sustainable groundwater use, administrators must employ remediation policies such as the pump-and-treat (P&T) method. The P&T method is primarily common and useful for decontaminating groundwater with highly soluble pollutants by pumping out and treating contaminated groundwater (Chu and Chang 2009b). Several studies have investigated the feasibility of coupling optimization technique with groundwater flow and transporting simulation to design P&T systems (Chang et al. 1992; McKinney and Lin 1994; Wang and Zheng 1998; Chang and Hsiao 2002; Chu et al. 2005; Chang et al. 2007). Significant advances over the past two decades apply optimized ground water management (Gorelick et al. 1984; Jones et al. 1987; Yeh 1992; Ahlfeld et al. 1988; McKinney and Lin 1994; Chang and Hsiao 2002; Hsiao and Chang 2002; Hsiao and Chang 2005; Chu and Chang 2010). However, the solution of the optimal groundwater contamination problem is computationally difficult because the nonconvexities inherent in the contaminant transport equation (Ahlfeld and Sprong 1998).

Strategic planning for groundwater remediation implicitly relies upon understanding the physical processes involved. Optimal remediation design is based on groundwater flow and pollutant transport simulation. Typical flow and pollutant transport models of contaminated aquifers predict the effectiveness of a single prospective pumping strategy in P&T remediation (McKinney and Lin 1994; Chang and Hsiao 2002; Hsiao and Chang 2005). Solving field-scale problems related to groundwater remediation design is time-consuming, as hundreds to thousands of numerical simulation runs may be required for searching optimal pumping strategies. However, the most well-calibrated simulation model is still a highly idealized representation of the real-world system because of the difficulties concerning accurate parameter estimation and simplifying model assumptions. One approach to save design time is to simplify the simulation model as much as possible, while retaining enough complexity so that it adequately reproduces system behavior.

Artificial neural network (ANN) which originated about several decades (McCulloch and Pitts 1943), were inspired by a desire to emulate human learning. The ANN is an alternative modeling and simulation tool and is proven to be highly effective for modeling nonlinear problem (Samani et al. 2007; Feng et al. 2008; Yesilnacar et al. 2008; Banerjee et al. 2011). Unlike traditional physical-based numerical models, an ANN often does not require explicit quantification and characterization of physical properties and conditions and are not based upon simplifying mathematical assumptions (Coppola et al. 2003a,b; Banerjee et al. 2011). Moreover, ANN models provide useful results without costly calibration time (Daliakopoulos et al. 2005; Feng et al. 2008). An ANN can effectively learn the system behavior of interest from representative data (Yesilnacar et al. 2008). Previous studies demonstrated an ANN methodology as a groundwater simulator in the optimization model. An ANN embedded within an optimization model can accurately predict ground water state in response to management alternatives (Rogers and Dowla 1994; Rao et al. 2005; Becker et al. 2006; Coppola et al. 2007; Chu and Chang 2009a). Rogers and Dowla (1994) used an ANN- Genetic Algorithm (GA) methodology to replace a traditional simulation-optimization model. The model used twenty pre-selected extraction locations with steady-state pumping and searched for the subset of wells producing the smallest volume of pumping water over a 40-year planning period. The ANN-GA methodology optimizes the set of pumping patterns for meeting remediation objectives (Rogers et al. 1995). Becker et al. (2006) coupled optimization and transport simulation models to three pump-and-treat systems for real problems. They used ANN-derived state transition equations to replace time-consuming simulation models in the optimization algorithm. Coppola et al. (2007) developed ANN with simulation data from a numerical ground water flow model developed for the study area. The ANNs were embedded into a multiobjective linear optimization model to find a compromise pumping policy that effectively balances the two conflicting objectives between water supply and wellfield vulnerability in the nearby contaminant area. Chu and Chang (2009a) integrated the ANNs and constrained differential dynamic programming (CDDP) for a groundwater resource-planning problem. The ANNs were used as surrogates of numerical models in groundwater flow simulation.

The above studies consider the fixed rates of pumping in the design problem and lack the insight between the dynamic operation, such as time-varying pumping rates, and operating costs. Remediation systems require a dynamic simulation or nonlinear optimization model in order to yield satisfactory results, unless the input assumptions justify a static system (Chang et al. 2007). Applying an optimization technique such as GA and simulated annealing (SA) to solve time-varying policies would dramatically increase required computational resources (Mckinney and Lin 1994; Wang and Zheng 1998; Rao et al. 2003). Accommodating these situations, an optimal dynamic groundwater remediation design is required to use constrained differential dynamic programming (CDDP) (Jones et al. 1987; Chang et al. 1992; Culver and Shoemaker 1992). Furthermore, the CDDP significantly reduces working dimensionality of the algorithm over that of mathematical programming algorithms, by taking advantage of the dynamic groundwater supply or water quality optimization problems through stage-wise decomposition (Hsiao and Chang 2002). Accordingly, the CDDP overcomes a serious limitation for conventional dynamic programming (DP) (Murray and Yakowitz 1979; Jones et al. 1987) and is efficient for solving time-varying management problems (Mansfield et al. 1998; Liu and Minsker 2001; Chang, et al. 2009). However, the computational work for CDDP model is proportional to the total number of state variables (Liao and Shoemaker 1991; Mansfield et al. 1998; Chang, et al. 2009). The significant increase in computational effort can be expected when using a fine mesh rather than a coarse mesh due to the nonlinearity and dynamic properties of this remediation strategy. Computational burdens that accompany field-scale problems hinder using the CDDP in actual remediation projects (Liu and Minsker 2001; Liu and Minsker 2002).

This study presents that the approach handles this optimization problem by effectively combining ANNs with the CDDP. The algorithm (ANN-CDDP) is a CDDP embedded with the ANNs. The ANN-CDDP computes optimal nonlinear time-varying pumping schemes to minimize the cost while meeting water quality-constraints. The embedded ANNs predict and evaluate system response, hydraulic head and contaminant concentrations under a series of pumping policies.

2 Formulation of the Proposed Management Model

The management model attempts to minimize the total cost of remediation composed of pumping and treatment system operating costs while meeting water quality-constraints (Chang et al. 1992). The dynamic optimal planning concerns with how to operate in the pumping wells at the most contaminated area. The remediation planning model is formulated as follows:

$$\min_{u_t^i, t=1,\ldots,T} J = \sum_{i \in I} \sum_{t=1}^{T} \left[a_1 u_t^i \left(L_*^i - h_{t+1}^i \right) + a_2 u_t^i \right] \tag{1}$$

subject to

$$\{x_{t+1}\} = T(x_t, u_t, t), \quad t = 1, 2, \ldots, T \tag{2}$$

$$c_N^j \le c_{\max}, \quad j \in \Phi \tag{3}$$

$$\sum_{i \in I} u_t^i \le u_{total}, \quad t = 1, 2, \ldots, T, \quad i \in I \tag{4}$$

$$u_{\min} \le u_t^i \le u_{\max}, \quad t = 1, 2, \ldots, T, \quad i \in I \tag{5}$$

where Eq. (1) represents the operating cost associated with network (I).The u_t^i denotes pumping rate at well I at time t and h_{t+1}^i denotes hydraulic head at well I at time t+1. $L_*^i(I)$ is the distance between the ground surface and the lower datum of the aquifer for each well. The expression $L_*^i - h_{t+1}^i$ simply represents drawdown at pumping well i. a_1 is the cost coefficient for pumping the contaminated groundwater, a_2 is the cost coefficient for the pumped water treatment. Equation (2) represents the system dynamics relation in the optimization and the transition equation. $x_t = [h_t : c_t]^T$ represents the continuous state variables representing hydraulic heads (h_t) and solute concentrations (c_t). In the study, the ANNs are used as the transition equations in nonlinear dynamic optimization. Equation (3) ensures the water-quality standard will be met at specified monitoring well j at the end of the planning period (t=N). Equation (4) specifies the capacity constraint for the treatment plants. The upper limit of Eq. (5) denotes each well capacity, while the lower limit can be applied to avoid well installation that has small pumping rates, which are obviously infeasible. $c_{\max}$ represents the maximum allowable concentration; u_{total} represents the maximum allowable treatment capacity from all extraction wells; $u_{\min}$ and $u_{\max}$ denote the minimum and maximum pumping rate for each well. I is an index set defining a pumping network ; Φ represents the set of observation wells.

3 Integration of CDDP and ANN

A hybrid model that integrates the ANNs with the CDDP solves the dynamic contaminant remediation problem as formulated by Eqs. (1) to (5). The following shows the procedure to develop the ANN-CDDP model (Chu and Chang 2009a), explained in more detail:

Step 1: Create training data by case simulations

The procedure generates data from case simulations performed by using ISOQUAD. ISOQUAD is a groundwater flow and contaminants transport simulation model for a confined two-dimensional aquifer (Pinder 1978). The transport model includes changes of contaminant concentration owing to advection, diffusion, dispersion, and the adsorption isotherm of aquifer (Chu and Chang 2009b). Numerical scheme applied in the model is the Galerkin finite element method for spatial integration and implicit finite difference for time integration. In the study, the total available data has been divided into two sets, training and validation set: 400 cases were used to train the ANNs, and 100 cases were used for validation. Each case is a series of simulations during the planning periods based on random pumping.

Step 2: Train ANNs to simulate hydraulic head and contaminant concentration

The ANN attempts simulation of brain (biological neural network). The network consists of an interconnected group of artificial neurons and processes information using a connectionist approach for computation. An ANN has two neural processing phases (Kumar 2004).

Learning is a process of adapting connection weights in an ANN to produce desired outputs. The recalling process attempts to retrieve information, based on weights obtained from the learning process, and predicts output data of the new example.

$$(h_{t+1}) = g_1(h_t, u_t), \quad t = 1, 2, \ldots, \mathrm{T} \tag{6}$$

$$(c_{t+1}) = \mathrm{g}_2(c_t, h_t, u_t), \quad t = 1, 2, \ldots, \mathrm{T} \tag{7}$$

In this study, two ANNs perform as groundwater flow and pollutant transport state transition equations, respectively (Fig. 1). Figure 1 (a) represents the groundwater flow ANN model, where the input state vector includes head and pumping rate at time t and the output state vector is the head at $t+1$. Equation (6) represents the the groundwater flow ANN model. The dimension of input state vector in Eq. (6) is $m+n$ and the output vector is n, where n is the number of observation well and m is the number of pumping well. For example, the groundwater flow ANN includes three inputs and two outputs if there are a pumping well and two observation wells in the case. Figure 1 (b) shows the ANN model for contaminant transport and indicates that the concentration at time $t+1$ is determined via the

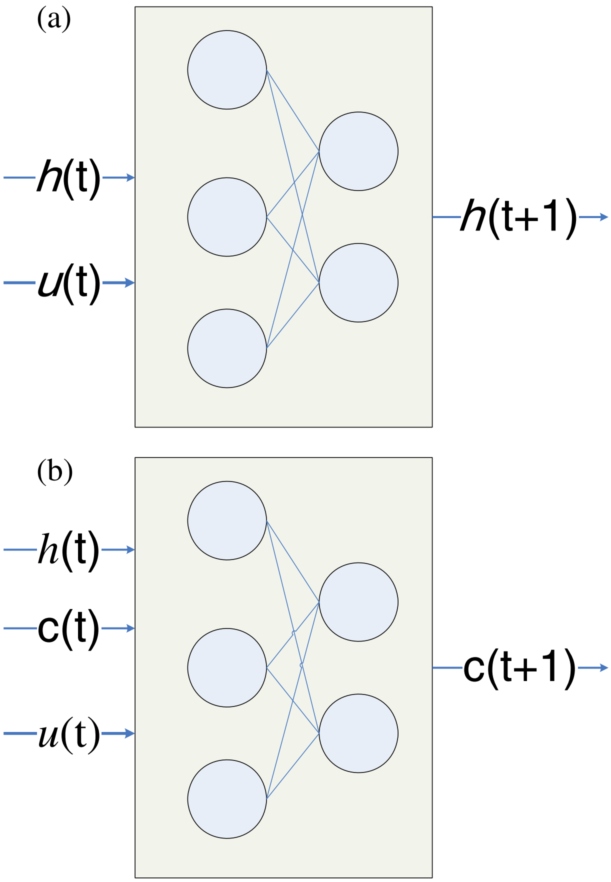

Fig. 1 **a** Groundwater flow ANN model (**b**) Contaminant transport ANN model

pumping rate, concentration, and hydraulic head at time t. Equation (7) is the input-output function in the contaminant transport ANN model, where the output, concentration at time $t+1$ (c_{t+1}), is a function of inputs, pumping rate (u_t), concentration (c_t) and hydraulic head (h_t) at time t. When predicting the concentration (c_{t+1}) for $t=1\ldots\mathrm{T}$, resulting from a pumping policy (u_t), the concentration (c_t) and the hydraulic head required (h_t) for $t=1\ldots\mathrm{T}$ in the contaminant transport ANN, Eq. (7). The dimension of input state vector in Eq. (7) is $2\,n+m$ and the dimension of output state vector is n. For example, there are five inputs and two outputs in the pollution transport ANN with one pumping well and two observations.

The back-propagation algorithm was used as the learning process in the multi-layer feed-forward network (Tsai and Lee 1999; MATLAB 2000; Pijanowski et al. 2002). The ANNs are trained using an ANN toolbox by the MATLAB 2000. In this model, a number of neurons are arranged in an input layer, two hidden layers with ten hidden neurons, and an output layer in the study. The activation functions (transfer function) for two hidden layers are hyperbolic tangents. In general, an ANN learns much faster when activation function is represented by a hyperbolic tangent (Negnevitsky 2002). Moreover, a network training function updates weight and bias values according to the Levenberg-Marquardt optimization (Gill et al. 1981). The algorithm will continue if the stopping criteria are not met. After training and validation, the ANN models are embedded with CDDP.

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

The ANN-CDDP is a successive approximation technique for solving optimal control problems, iteratively determining the optimal solution to the problem stated in Eqs. (1) to (5). The objective function depends upon control and state variables with identical time index (t). Equation (2) is the transition function to simulate system response induced by the control policy, the groundwater flow and pollution transport ANN models (Eqs. (6) and (7)) The ANN-CDDP computes the optimal solution by resolving a series of quadratic problems, the quadratic approximation of the original problem in Eqs. (1) to (5). Through the backward and forward sweeps, the ANN-CDDP searches the optimal policy and determines the minimal operating costs.

The CDDP algorithm is employed in the backward and forward sweeps to resolve the series of sub-problems. In the backward sweep, an update control policy is evaluated through solving a series of sub-problems that require the variable derivative values (Chang et al. 1992; Hsiao and Chang 2002). The derivatives of the transition equation (Eq. (2)), the ANN models (Eqs. (6) and (7)) in this study, are obtained by chain rule (Dimopoulos et al. 1995; Chu and Chang 2009a). Derivative of transition equation with respect to x_t, u_t is:

$$\left[\frac{\partial T}{\partial x_t}\right] = \left[\frac{\partial x_{t+1}}{\partial x_t}\right] = \begin{bmatrix} \frac{\partial h_{t+1}}{\partial h_t} & \frac{\partial h_{t+1}}{\partial c_t} \\ \frac{\partial c_{t+1}}{\partial h_t} & \frac{\partial c_{t+1}}{\partial c_t} \end{bmatrix} \tag{8}$$

$$\left[\frac{\partial T}{\partial u_t}\right] = \left[\frac{\partial x_{t+1}}{\partial u_t}\right] = \begin{bmatrix} \frac{\partial h_{t+1}}{\partial u_t} \\ \frac{\partial c_{t+1}}{\partial u_t} \end{bmatrix} \tag{9}$$

For a multilayered network, the derivatives in the transition equation are derived by ANN in the following (Chu and Chang 2009a).

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

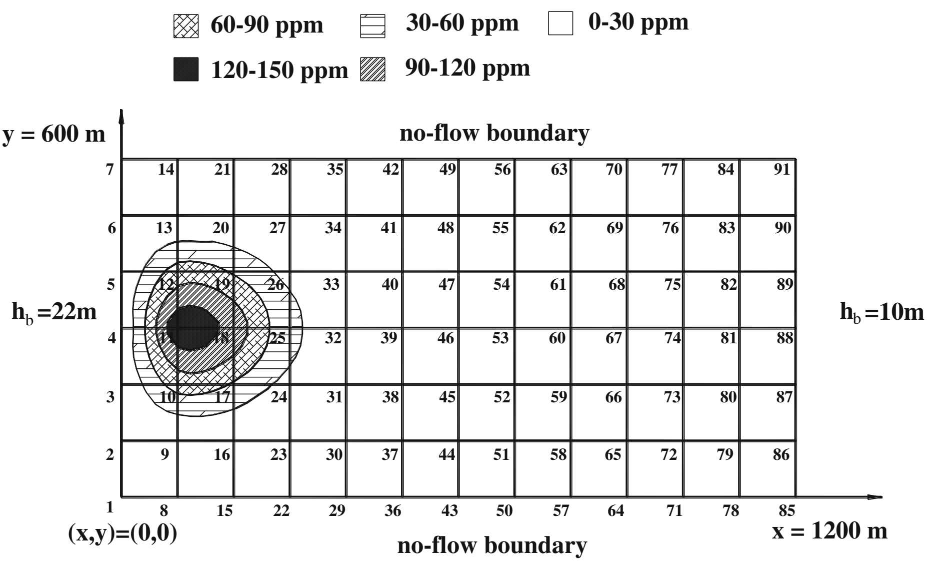

Fig. 2 Finite-element mesh, boundary conditions, and initial plume in Case 1

where O_k (i.e. h_{t+1}, c_{t+1} in the algorithm) denotes the output for node k in the output layer; jn, $jn-1,\ldots$, and $j1$ denote the neural units in the nth, $n-1th,\ldots$, and 1st hidden layer; O_i (i.e. h_t, c_t, u_t) denotes the input for node I in the input layer; f is transfer function; $net_j = \sum_i w_{i,j}O_i - b_j$; j=k, jn, $jn-1,\ldots$, and $j1$, $w_{i,j}$ 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.

The algorithm in the forward sweep computes updated policy using feedback function and performs the ANN to determine latter system state at each time step. Quadratic programming is applied to solve the series of quadratic sub-problems for t=1…T, forward in time, and obtains the optimal policy. Notably, the computed optimal policy becomes the nominal policy for the next iteration (Chang and Hsiao 2002; Chang et al. 2007). Since a quadratic problem is only an approximation of the original problem, iterations are required.

Table 1 Aquifer properties and simulation parameters of cases

Parameter	Value
Hydraulic conductivity	4.31×10^{-4} m/s
Longitudinal dispersivity	70 m
Transverse dispersivity	3 m
Diffusion coefficient	1×10^{-1} m^2/s
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	10 m
Ground elevation	120 m

Table 2 Management model parameters and cost coefficients

Parameter	Value
Maximum allowable treatment capacity (u_{total})	150 L/s
Maximum pumping rates ($u_{\max}$)	100 L/s
Minimum pumping rates ($u_{\min}$)	0 L/s
Maximum allowable concentration ($c_{\max}$)	$0.5 mg$/L
Cost coefficient a_1	\$1000 /(m^3/s·Δt)
Cost coefficient a_2	\$40000 /(m^3/s·Δt)
Period length (Δt)	91.25 day
Period number	20

Moreover, Murray and Yakowitz (1979), Jones et al. (1987), and Chang et al. (1992) provided a detailed discussion of the CDDP algorithm.

4 Results and Discussion

4.1 Case1: Comparison of the Results of Various Pumping Wells

This study performs numerical analyses on a hypothetical groundwater remediation problem to verify effectiveness of the proposed methodology. The procedure adapted a groundwater remediation problem from the example in Chang and Hsiao (2002). Figure 2 displays a hypothetical confined aquifer with dimensions of 600 m by 1200 m to demonstrate algorithm performance described above. The boundary conditions on the north and south sides are no-flow boundaries for head and concentration. Constant-head boundaries with 22 m and 10 m are located on the west and east sides individually, and constant-concentration boundaries with 0 mg/L are located on both sides. The aquifer properties and simulation parameters are listed in Table 1. The initial peak concentration within the aquifer is 150 mg/L, and the water quality goal at the end of five years must not exceed 0.5 mg/L at all the observation wells. Twenty management periods are included in the procedure and each period (Δt) is 91.25 days. The management model parameters associated with the constraints and cost coefficients are listed in Table 2.

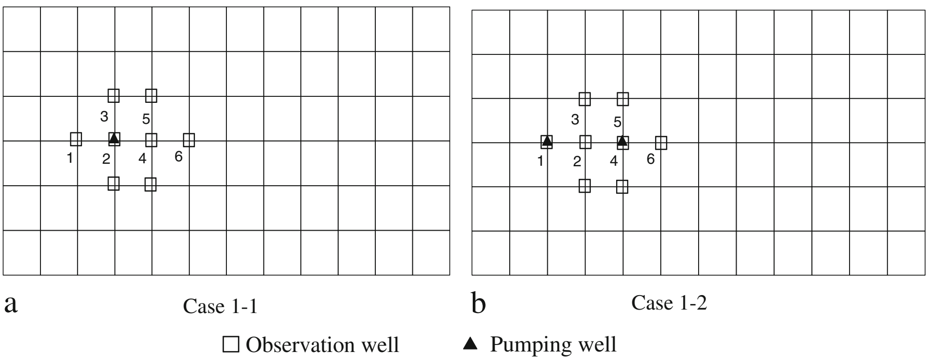

Fig. 3 Remediation system design of Case 1-1 and Case 1-2

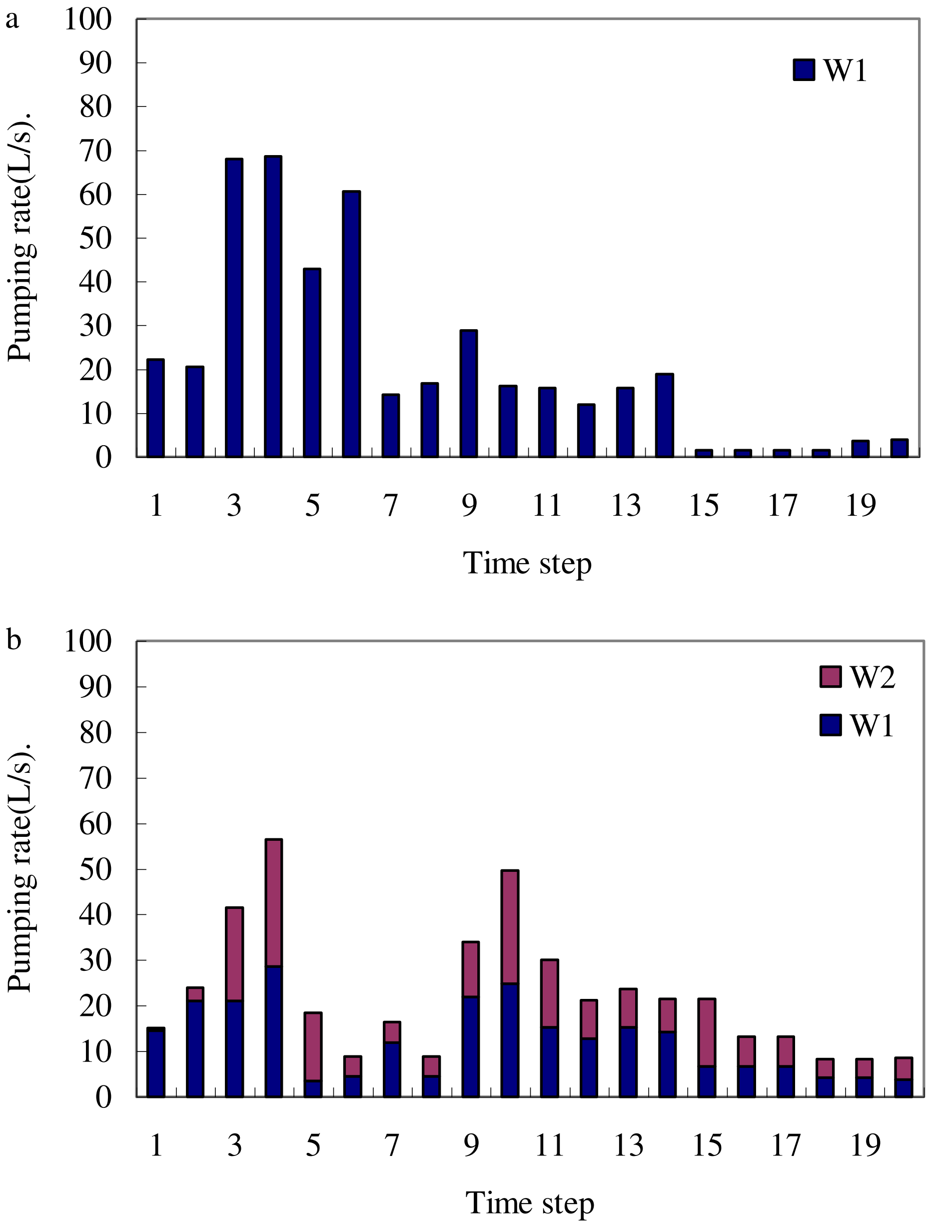

Fig. 4 Optimal pumping rates at each period in (**a**) case 1-1, (**b**) case 1-2

Figure 3 shows the plan view of Case 1-1 with one pumping well (black triangle), eight observations (open square) and Case 1-2 with two pumping wells and eight observations. Owing to the symmetrical condition of this study, only six observation wells need to be considered. The inputs and outputs of the ANNs depend on the information from pumping and observation wells. In groundwater flow ANN, the input vector includes hydraulic heads and pumping rate at time t and the output vector is the hydraulic heads at $t+1$. In the

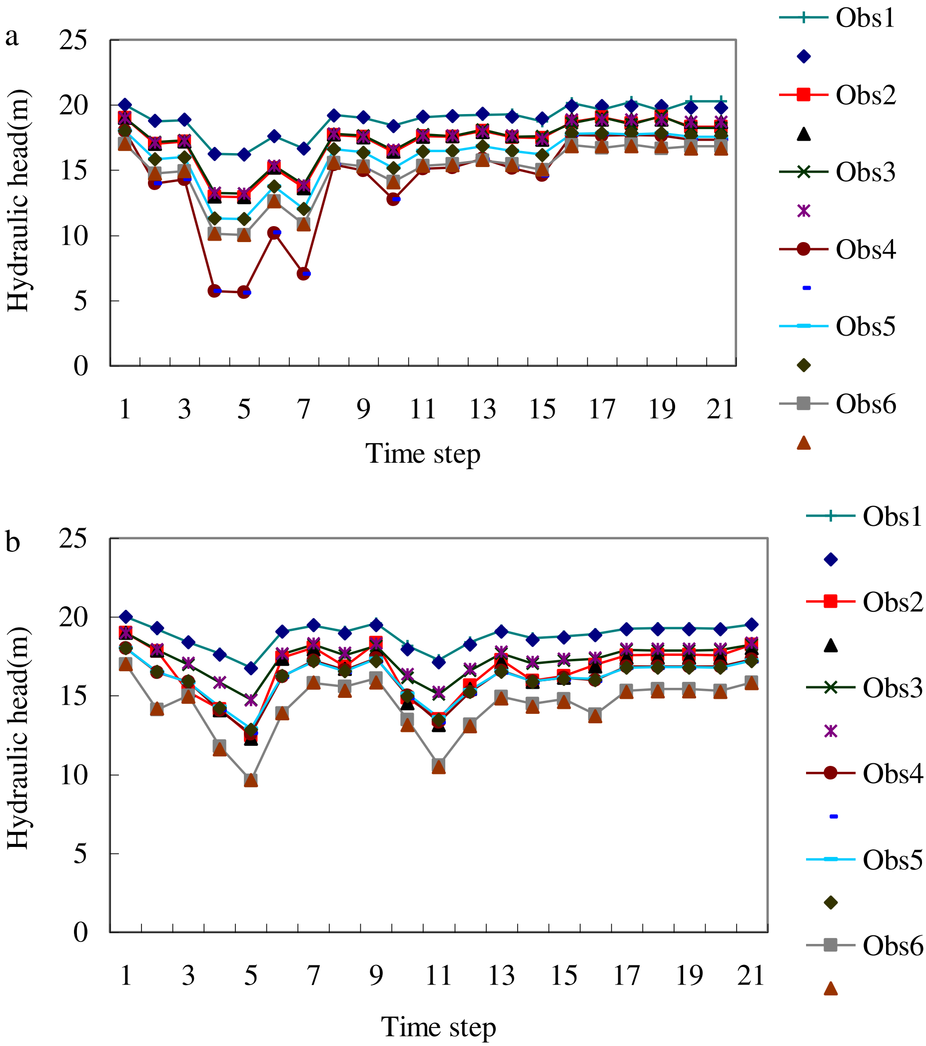

Fig. 5 Hydraulic head at each period in (**a**) case 1-1, (**b**) case 1-2

contaminant transport ANN, the inputs are pumping rate, concentration, and hydraulic head at time *t* and the outputs are the concentration at *t+ 1*. The typical processes of the ANN parameters identification such as the hidden layer number and the neuron number are listed in Negnevitsky (2002) and Kumar (2004). The following demonstrates the influence of neuron number in the ANN. The contaminant transport ANN is more complicated than the groundwater flow ANN, so the contaminant transport ANN is taken as the example for demonstration. In the cases, the average CPU time for training cases is 531 s in two hidden layers with five neurons and the ANN root mean squared error (RMSE) is 0.270 ppm. The average CPU time for the cases is 3,210 s and the RMSE of the ANN with ten neurons in two hidden layers is 0.106 ppm. The average CPU time for cases with twenty neurons is 9,590 s and the RMSE increases to 0.120 ppm. Thus, ten hidden neurons are used in the network to ensure a balance of both accuracy and computation effort. The relative validation

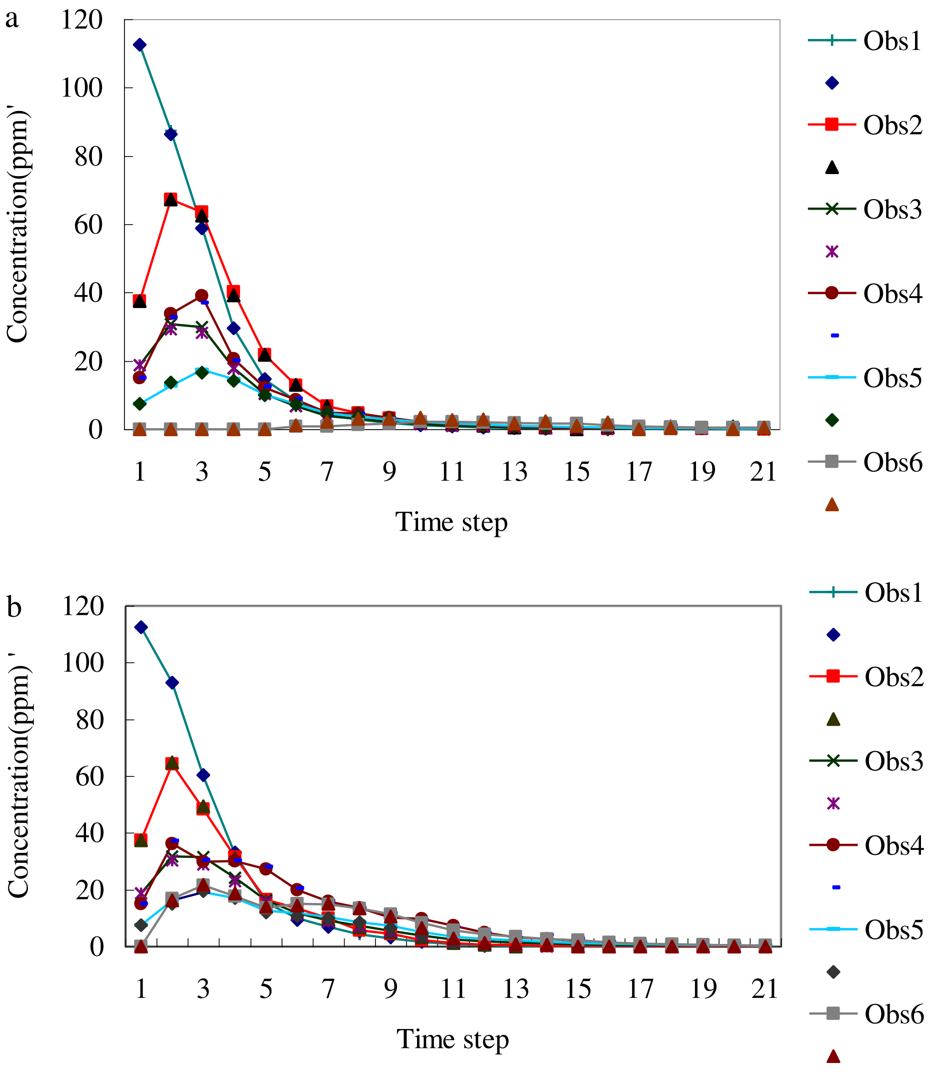

Fig. 6 Concentration at each period in (**a**) case 1-1, (**b**) case 1-2

errors with respect to average hydraulic head and concentration are less than 0.02% and 0.5% for the validation data sets, illustrating high predictive performance. Additionally, the accuracy of the ANN for predicting hydraulic heads and concentrations will be demonstrated with the following case studies.

Table 3 Comparison of ANN-CDDP and ISOQUAD-CDDP solutions in Case1

	Pumping well number	Optimal cost using ANN-CDDP	Optimal cost using ISOQUAD-CDDP	Relative error (%)
Case 1-1	1	$69,652	$68,174	2.16
Case 1-2	2	$68,845	$68,533	0.45

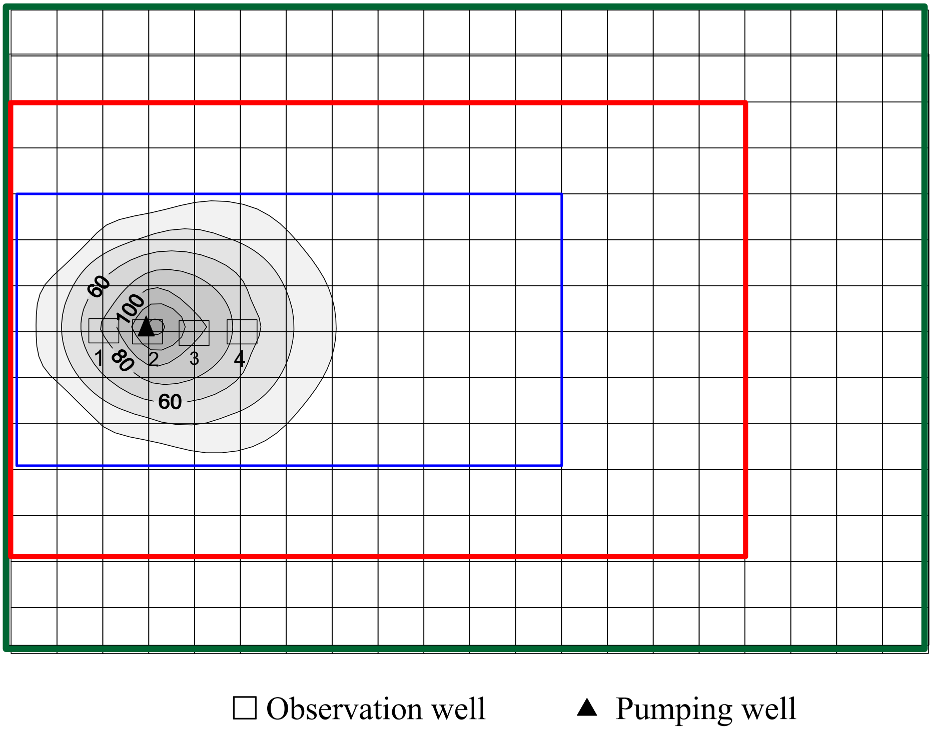

Fig. 7 Plan view of Cases 2-1(blue), 2-2 (red) and 2-3 (green)

In Case 1-1 and Case 1-2, these cases are different in the well locations and numbers. Optimal pumping rates in Case 1-1 and Case 1-2 are determined by ANN-CDDP, shown as Fig. 4 (a) and (b). Hydraulic heads at each period are varied with pumping rate (Fig. 5 (a) and (b)). Concentration variations during remediation period are shown in Fig. 6 (a) and (b). The symbols represent hydraulic head and concentration of ANNs while the line represents the ISOQUAD simulations under the same condition. Results show the ANN and ISOQUAD solutions for hydraulic head and concentration under the optimal pumping rate are similar. For these cases, there is a good fit between the ANN and ISOQUAD. The ANN is trained with the simulation data to predict ground water level at various locations under variable pumping conditions (Coppola (2000)). The groundwater level at next time is forecasted based on the management alternatives. The study demonstrates that an ANN can be trained to accurately predict hydraulic head and concentration under pumping. The results reveal that this ANN technique performs close to conventional simulations and achieves an equally high degree of predictive accuracy. The ANN greatly simplifies the

Table 4 Three case-study sizes in Case 2

	Number of nodes	Number of elements	Number of state variables
Case 2-1	91	72	77
Case 2-2	187	160	165
Case 2-3	315	280	285

Table 5 Comparison of ANN-CDDP and ISOQUAD-CDDP solutions in Case2. Optimal operating cost

	ANN-CDDP	ISOQUAD-CDDP	Relative error (%)
Case 2-1	\$104,454	\$103,264	1.14
Case 2-2	\$107,112	\$103,099	3.75
Case 2-3	\$109,221	\$103,260	5.45

complex dynamics inside when compared to using simulation models. Besides, optimal operating cost in ANN-CDDP and ISOQUAD-CDDP is illustrated in Table 3. Proposed model (ANN-CDDP) accuracy can be quantified when compared with ISOQUAD-CDDP (Chang et al. 1992; Culver and Shoemaker 1992). The cost results demonstrate that relative error is 2.16% or less. Therefore, the case verifies the feasibility of the ANN-CDDP. The ANN-CDDP is an alternative for dynamic optimal groundwater quality management. Furthermore, containing the contamination by removing contaminated ground water should be a dynamic process. Dynamic policies which allow changing pumping policies as the contaminant plume moves, would expectedly be more cost-effective than static policies (Chang et al. 1992, 2007).The optimal remediation system is cost-effective and the time-varying operation policy is allowed to change as the contaminant plume moves.

4.2 Case2: Comparison of the Influence of Various Domain Sizes

This study presents the optimal solutions for three hypothetical, isotropic, confined aquifers with different dimensions: 600 m by 1200 m (Case2-1: blue), 1000 m by 1600 m (Case2-2: red) and 1400 m by 2000 m (Case2-3: green). The three different domains with finite-element mesh, along with one pumping well (black triangle) and four observation wells (open square) are shown in Fig. 7. Table 4 lists the number of finite-element nodes and elements in the cases. The boundary conditions, initial conditions, and time scale are the same for both Case 1 and Case 2. The aquifer properties and simulation parameters also are listed in Table 1.

The ANN training data are generated independently from the simulation results based on different domain sizes. After training and validation, ANNs are embedded in CDDP and the current study compares the present operating cost value under various cases between ANN-CDDP and ISOQUAD-CDDP. Table 5 illustrates the operating costs of the optimal policy. Results also show that the cost difference between ISOQUAD-CDDP and ANN-CDDP in three various cases is 5.45% or less. However, Table 6 indicates that the difference of computational work is related to domain size. Result provides information to support for the hypothesis that computational work for the ISOQUAD-CDDP is proportional to O (Ns^{3}),

Table 6 Comparison of ANN-CDDP and ISOQUAD-CDDP solutions in Case2. CPU time (unit: Sec)

		ANN-CDDP	ISOQUAD-CDDP	Ratio
Case 2-1	CPU time	84.37 (7)	33.22 (14)	1/0.4
	CPU time each iteration	11.32	2.37	1/0.2
Case 2-2	CPU time	160.92 (15)	148.70 (13)	1/0.9
	CPU time each iteration	10.62	11.90	1/1.1
Case 2-3	CPU time	130.57 (15)	1659.16(11)	1/12.7
	CPU time each iteration	8.43	150.83	1/17.9

() iteration number

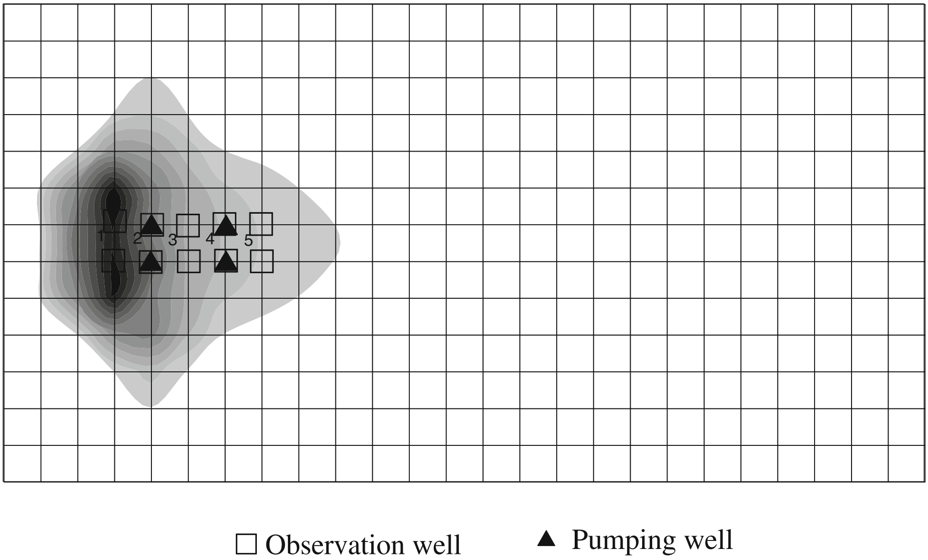

Fig. 8 Plan view of Case 3

where *Ns* is the total number of state variables (Mansfield et al. 1998). However, the ANN including few representative state variables is applied as a response function for the aquifer system. From the cases results, the computational loading for ANN-CDDP does not increase with domain size. Particularly, case 2-3 presents a comparative table involving ISOQUAD-CDDP and ANN-CDDP and shows that the latter saves significant computational time. The ANN-CDDP computational time is as little as 1/17.9 when compared to the ISOQUAD-CDDP.

4.3 Case3: A Fine Mesh Problem

This study presents the ANN samples obtained for a fine mesh problem with dimensions of 650 m by 1250 m to demonstrate the ANN-CDDP algorithm performance described below. Figure 8 shows the finite-element mesh with 364 finite-element nodes and 336 active state variables. The site includes four pumping wells (black triangle) and ten observation wells (open square). Owing to the symmetrical condition of this study, only two pumping wells and five observation wells should be considered. The boundary conditions on the north and south sides are no-flow boundaries for head and concentration. Constant-head boundaries with 42 m and 30 m are located on the west and east sides individually, and constant-concentration boundaries with 0 mg/L are located on both sides. This study assumes the initial condition of the hydraulic head distribution prior to pumping to be steady state. The initial peak concentration within the aquifer is 120 mg/L, and the water quality goal at the end must be limited to 0.5 mg/L at all observation wells. The planning horizon is divided

Table 7 Comparison of ANN-CDDP and ISOQUAD-CDDP solutions in Case 3. Optimal operating cost

	ANN-CDDP	ISOQUAD-CDDP	Relative error (%)
Optimal operating cost	$462,906	$441,636	4.81%

Table 8 Comparison of ANN-CDDP and ISOQUAD-CDDP solutions in Case 3. CPU time (unit: Sec)

	ANN-CDDP	ISOQUAD-CDDP	Ratio
CPU time	133.375 (14)	10236.30 (40)	1/76.7
CPU time each iteration	9.65	255.90	1/26.5

() iteration number

into twenty periods and the time between each period in the management model (Δt) is 10.2 days. The aquifer properties and simulation parameters are illustrated in Table 1.

ANN models are trained using the above-described procedures and then ANN-CDDP finds the near-optimal solutions when compared to ISOQUAD-CDDP. Tables 7 and 8 illustrates the comparison of optimal policy cost and computational time between ANN-CDDP and ISOQUAD-CDDP in Case 3. Results imply that the optimal operating cost difference between ANN-CDDP and ISOQUAD-CDDP is 4.81%. Many researchers have successfully applied the ANN for regional groundwater level simulations in the field data (Coppola et al. 2003b; Feng et al. 2008).The study incorporates the ANNs into the CDDP and the system is reduced to few representative control points by using the ANNs. Enforcing the computational time reduction in the design potentially enhances comprehensive concerns in the dynamic decision process but increases a little cost. However, the suggested pumping policy is a good reference and fast response for decision making. Although the ANN-CDDP policy is not optimal, it is more computationally efficient than the traditional model. In the site operation, the model uncertainty could be compensated by the observation data through feedback. A practical remediation system requires the effective planning model for an appropriate usage. The ANN-CDDP is a good choice because it reduces computational time each iteration by as much as 1/26.5 compared to the time required by the ISOQUAD-CDDP in the case of 364 nodes. Compared with previous studies, the multiscale method (Liu and Minsker 2001) reduces the computational time of each iteration by 0.53 in the case of 429 nodes; the sparsity (Mansfield et al. 1998) method reduces the computational time of each iteration by 0.31 in the case of 500 nodes. Accordingly, it is demonstrated that ANN-CDDP obtains better results than these methods. Comparison implies that the ANN-CDDP computes optimal operating cost efficiently. Although the model error increases slightly, computational time relating to ANN-CDDP remains economical in the large-field case. Future work will consider applying the ANN to field-site cases in the remediation planning.

5 Conclusions

This study proposes a novel optimization scheme for nonlinear dynamic groundwater quality management. The proposed model integrates a neural network (ANN) with constrained differential dynamic programming (CDDP) to determine optimal time-varying operations in groundwater remediation planning. Specifically, a trained ANN is embedded with the derivative-based CDDP optimization technique. Applying an ANN as a transition function greatly simplifies the complex dynamics involved in simulation models. This study uses the ANN-CDDP to determine dynamic optimal operating costs for a specified network. This approach benefits groundwater remediation planning by training neural networks to predict results based on a few representative wells. It is an efficient procedure for determining dynamic pumping rates at each well, and its optimal operation strategy effectively controls contaminant plumes.

The proposed methodology reduces the computational time and complexity of large-field case compared to the conventional models. The computational time of the ANN-CDDP for a case involving 364 nodes is 1/26.5 of the time required by the conventional model (ISOQUAD-CDDP). Large-field problems may considerably increase the number of state variables, greatly increasing the complexity of optimization. By embedding ANN into the optimization model, the proposed methodology can handle large-field problems using representative observed states, irrespective of domain sizes. Future studies should apply field data to train the ANN, revealing the details of a real-world remediation case.

Acknowledgement Ann Yu and Wallace Institute are appreciated for its editorial assistance. The authors would like to thank the editors, reviewers, Dr. Chen, Prof. Shan and anonymous helpers for their contributions to this study.

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