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The Use of Neural Networks and Genetic Algorithms for Design of Groundwater Remediation Schemes

Zheng-fu Rao and D. G. Jamieson

Department of Civil Engineering, University of Newcastle upon Tyne, Newcastle upon Tyne, NE1 7RU, UK

Abstract

The increasing incidence of groundwater pollution has led to recognition of a need to develop objective techniques for designing remediation schemes. This paper outlines one such possibility for determining how many abstraction/injection wells are required, where they should be located etc., having regard to minimising the overall cost. To that end, an artificial neural network is used in association with a 2-D or 3-D groundwater simulation model to determine the performance of different combinations of abstraction/injection wells. Thereafter, a genetic algorithm is used to identify which of these combinations offers the least-cost solution to achieve the prescribed residual levels of pollutant within whatever timescale is specified. The resultant hybrid algorithm has been shown to be effective for a simplified but nevertheless representative problem; based on the results presented, it is expected the methodology developed will be equally applicable to large-scale, real-world situations.

Introduction

The widespread occurrence of problems associated with subsurface contamination has resulted in the development of various methodologies for groundwater remediation. In designing practical programmes to restore aquifers which are contaminated by leachates from landfills, illegal tipping or accidental spillages, groundwater-resource managers face a wide range of technical options. The choice of which method is best for a given site is a multi-step decision-making process that seeks to define, implement and operate the most appropriate and economical solution to restore groundwater quality to the standards set by the regulatory agency.

Probably the most common method of groundwater remediation that has been applied in practice is the so-called 'pump-and-treat' system (Bardos, 1994); the abstraction well field is configured to contain and subsequently remove the contaminant plume from the aquifer. Once the flow rate and contaminant concentrations of the extracted water are determined, a treatment system can be designed to remove enough of the contaminants to meet the effluent-quality standards suitable for reinjection or discharge to the nearest watercourse. When reinjection is used to dispose of the effluent, an injection well field needs to be designed to aid the process of isolating the plume hydraulically as remediation proceeds. Obviously, the treatment system used to remove contaminants from the groundwater, the abstraction well field and reinjection well field are intimately inter-related. Even though this technology has been developed extensively, it is still difficult to design a system that will minimise the amount of water recirculated within the contaminated region during the remediation process (Hoffman, 1993).

When designing a pump-and-treat remediation system, a manager must decide, among other things, how many remediation wells to install, where to locate the wells and what pumping rate to assign to each well. On a more objective basis, this problem can be defined as the selection of optimal number, location and pumping rates for the remediation wells, so that the prescribed residual level of contaminant is achieved within a given period of time. This requires the formulation of mathematical models which simulate both groundwater flow and contaminant transport, making it possible to predict the effects of pumping on contaminant movement under various conditions. Moreover, some form of optimization procedure needs to be incorporated to operate in conjunction with the simulation model, if an optimal solution is to be achieved.

In the past, conventional optimization methods have been used for the design of groundwater remediation schemes and there exists a large body of literature related to the applications (Gorelick, 1983; Yeh, 1992; Wagner, Shamir and Hemati, 1992; Ahlfeld *et al.* 1995). Typically, groundwater remediation system designs are formulated as a mixed-integer programming model involving both continuous and integer variables. These formulations have included mixed-integer linear (MILP) and nonlinear programming (MINLP) in which the selection of well locations is regarded as integer decision-variables and the assignment of pumping rates as continuous decision-variables. Willis (1976) used MILP to determine the optimal treatment processes associated with a well field for the disposal, by underground injection, of municipal wastewater effluent after treatment. Linear programming was used by Lefkoff and Gorelick (1986) in which pumping, injection and treatment costs were considered. Here, a linear treatment-cost function was used which essentially models the cost of a generic solution rather than the actual physical process. This approach is equivalent to a multiobjective programming problem using weighting functions which shift the solution from a well field cost-dominated solution to a treatment cost-dominated solution. In their dynamic programming method, Culver and Shoemaker (1992) assumed treatment costs were linearly related to abstraction rate but capital costs were not considered. However, Lee and Kitanidis (1991) included both capital and operation costs of treatment, pumping and injection in an optimal control formulation of the pump-and-treat design problem. Sawyer and Ahlfeld (1995) used MILP to minimize the cost of installing and operating a large-scale hydraulic plume containment scheme. The cost function included fixed and simplified linear costs of well installation and operation, respectively. Karatzas and Pinder (1994) approximated the discontinuous fixed charges by an exponential penalty coefficient and used an outer-approximation method to solve a concave nonlinear problem. Apart from the mixed-integer nonlinear formulation, these problems typically exhibit non-convexities and multiple, locally optimal solutions.

Owing to the difficulties in handling integer variables in the mixed-integer linear and nonlinear problem, groundwater remediation design problems are frequently simplified by neglecting the discontinuous variables associated with the fixed costs of installing wells and treatment systems which are assumed to be small in comparison with the pumping costs over a prolonged period. When the integer variables are neglected in the formulation, the methods often reduce to a standard nonlinear problem which can be solved by nonlinear programming (Gorelick *et al.*, 1984; Ahlfeld, 1990). These methods employ gradient-based algorithms to adjust decision variables so as to optimize the objective function of the model. Such algorithms require computing the sensitivities of state variables, e.g., head or concentration, at certain locations. Sensitivities are difficult to programme, as in the case of the adjoin-sensitivity method, or computationally expensive to generate, as in the case of perturbation methods and in general, are not particularly robust. Furthermore, the cost functions of typical groundwater system components may be either discontinuous or highly complicated, making it difficult to calculate or estimate the derivatives of these functions with respect to the decision variables. As a result, there is no guarantee that a global optimum of a groundwater remediation design model will be found by non-linear programming methods.

Concerns about the computational burden associated with field-scale applications, global optimality and the difficulty of handing discontinuous variables have led some researchers to continue seeking improved methods for optimising the design of groundwater remediation schemes. In recent years, for solving complex optimization problems, alternative algorithms have been developed that are applicable to groundwater management problems, including combinatorial optimization methods such as genetic algorithms (McKinney and Lin, 1994; Rogers and Dowla, 1994), simulated annealing (Dougherty and Marryott, 1990; Kuo *et al.*, 1992; Marryott *et al.*, 1993), and neural networks (Ranjithan *et al.*, 1993; Rogers and Dowla, 1994), etc. These new methods all have a high degree of inherent parallelism and are readily adaptable to massively-parallel computers.

This paper demonstrates the applicability of a hybrid artificial neural network and genetic algorithm for optimising the system design of a groundwater pump-and-treat remediation scheme. Once the potential sites for remediation (abstraction and injection) wells have been identified, an artificial neural network is used to conjunction with a groundwater flow and contaminant-transport simulation model to capture the knowledge for predicting the effectiveness of different combinations of abstraction/injection sites. Thereafter, a genetic algorithm is used to identify the optimal pumping regime, with a view to determining the most cost-effective solution for achieving the prescribed residual level of pollutant within whatever timescale is specified.

Groundwater Remediation Design

OPTIMIZATION MODEL FOR GROUNDWATER REMEDIATION DESIGN

In most cases, pumping greater amounts of water adds to the expenses of remediation. Therefore, the sum of pumping rates is frequently used as the measure of remediation efficiency, or surrogate for costs, and taken to be the objective of the optimization models. The sum of pumping volumes is another commonly used objective function. Both these objective functions assume a linear relationship between the amount of water pumped and the cost of remediation. Other possible choices for the objective function are the time of cleanup, pumping costs, well construction costs, water treatment costs, or some combination of these. It is also possible to consider maximization of contaminant removal. Here, the goal of the remediation is often incorporated into the constraints of the optimization model. Possible remediation goals are hydraulic containment of the plume, complete removal of detectable contamination, or prevention of increases in down-gradient contaminant concentrations above a chosen level.

As mentioned previously, the integer variables associated with fixed costs of installing wells are frequently omitted from the models, implying that the costs associated with these factors are small when compared with long-term operating costs (Ahfeld, 1990). The resulting designs have been defended as appropriate for remediation problems where plumes are ill-defined and cleanup periods are long, since inefficient wells can be removed or relocated after a time. This simplification can lead to designs that rely on a large number of wells pumping at small rates over long time periods. However, in an era when remediation costs are increasing exponentially and remediation periods are progressively shorter, as a result of chemical, physical, and biological enhancements to pump-and-treat systems, these simplifications are no longer warranted and may lead to inefficient and ineffective system designs as these fixed costs may have a significant effect on the optimal design.

If the objective function of the design model is to minimize the total cost of pump-and-treat remediation of a contaminated aquifer, including the capital and operating costs of the treatment system in addition to the abstraction and injection well fields, the conventional approach would have been to use a mixed-integer nonlinear model in which the total cost is defined as:

C = Cost of abstraction and treatment
+ Cost of injection
+ Cost of well installations and treatment plants

Thus, the formulation of the optimal groundwater remediation model may be expressed mathematically as follows:

$$\underset{y,q}{\text{Min}}\left\{F(q,y)=\sum_{i\in E\cup I}[f_i(q_i)+C_i y_i]\right\} \tag{1}$$

Where C_i is the net present value of the cost for abstraction facilities (inclusive of treatment) or injection well installation; $f_i(q)$ is the net present value of the cost function for abstraction well and treatment operations or for injection well operation; I is the number of wells that can be considered as remediation wells for injection; E is the number of wells that can be considered as remediation wells for abstraction; $q = (q_1, q_2, \ldots, q_{E+I})$, q_i is the abstraction or injection pumping rate at location i; $y = (y_1, y_2, \ldots, y_{E+I})$, y_i is a binary variable indicating whether the well is selected at location i which, if selected as a pumping site $y_i = 1$, otherwise $y_i = 0$.

It is assumed that each potential remediation well site either for abstraction or injection is predefined; thus the total number of well sites is $N = E + I$. Therefore, Eqn.. (1) can be rewritten as:

$$\underset{y,q}{\text{Min}}\left\{F(q,y)=\sum_{i=1}^{N}\{f_i(q_i)+C_i y_i\}\right\} \tag{1}$$

The constraints within the design model include the following:

(1) Upper bound on concentration at regulatory compliance points in the aquifer at the end of the remediation period (0, T)

$$c_{jT}(q) \le c^* \quad j \in \Omega_c \tag{2}$$

where $c_{jT}(q)$ is the concentration in the aquifer at location j at the end of the remediation period; the computation of $c_{jT}(q)$ requires evaluation of the dynamic simulation model to time T; c^* is residual level of pollutant prescribed by the regulatory authority; and Ω_c is a set of locations where compliance standards are enforced.

(2) Upper and lower bounds on the abstraction and injection rates

$$y_i q_i^{low} \le q_i \le y_i q_i^{up} \quad i = 1, 2, \ldots, N \tag{3}$$

where q_i^{low} and q_i^{up} are lower and upper pumping rate bounds, respectively.

GROUNDWATER FLOW AND CONTAMINANT TRANSPORT SIMULATION MODEL

The movement, accumulation, and transformation of a contaminant in an aquifer can be predicated by a simulation model approximating the governing flow and mass transport equations. For the purpose of groundwater remediation design, the simulation model is employed to evaluate the effects of alternative remediation (abstraction and injection) strategies on hydraulic heads and contaminant concentrations at particular locations.

Changes in the aquifer hydraulics as a result of pumping (abstraction and injection) are assumed to be rapid compared to corresponding changes in contaminant concentration, so steady-state flow conditions are assumed in the aquifer during remediation. If confined flow is assumed, the physics of the groundwater system can be captured using a vertically-averaged (two-dimensional) representation of the coupled partial differential equations describing fluid flow, velocity and solute transport (Bear, 1972):

$$\frac{\partial}{\partial x_j}\left(bK_{jk}\frac{\partial h}{\partial x_k}\right)+\sum_{i=1}^{N}q_i\delta(n_i)=0 \tag{4}$$

$$v_j = -\frac{K_{jk}}{\phi}\frac{\partial h}{\partial x_k} \tag{5}$$

$$\frac{\partial}{\partial x_j}\left(D_{jk}\frac{\partial c}{\partial x_k}\right)-v_j\frac{\partial c}{\partial x_j}+\frac{1}{b\phi}\left(\sum_{i=1}^{N}q_i(c-c_i^q)\delta(n_i)\right)=R\frac{\partial c}{\partial t} \tag{6}$$

where Einstein's convention for tensor notations applies to the indices j and k (j, k = 1, 2 designates the two-dimension coordinates, x_1, x_2, respectively); b is saturated thickness of the aquifer; h is vertically averaged hydraulic head; K_{jk} is hydraulic conductivity tensor; N is the total number of locations for abstraction/injection wells in the aquifer; D_{jk} is tensor of hydrodynamic dispersion coefficients; q_i is pump rate (< 0 for abstraction or > 0 for injection) for pumping well i located at node point, n_i; $\delta(n_i)$ is Dirac delta function evaluated at nodal point, n_i; R is retardation coefficient; v_j is j-direction component of groundwater pore velocity; ϕ is porosity of aquifer medium; c is contaminant concentration in the aquifer; c_i^q is the contaminant concentration in water injected or abstracted by well i.

Equation (4) describes the changes in hydraulic head distribution over time as a result of boundary conditions, abstraction and injection rates, and the values of head at the beginning. Equation 5 is Darcy's law by which the seepage velocity is calculated. Equation 6 is a solute mass balance which describes spatial redistribution of solute due to advection, dispersion, and retardation. The governing equations are usually discretised using a Petrov-Galerkin finite-element method for the spatial derivatives and an implicit finite-difference approximation for the temporal derivations.

In the context of groundwater-remediation design, the parameters in Eqns (4)–(6) that are considered to be controllable are the pump rates q_i and pump locations, n_i, $i = 1, 2, \ldots, N$. These parameters serve as the decision-variable with n_i implicitly constrained to lie within a set of predefined nodal locations. All other aquifer parameters are assumed known from model calibration.

Mapping Groundwater Flow and Contaminant Transport Simulation Using ANNs

Having described a groundwater remediation optimization model as defined by Eqns (1)–(6), it is evident there would be substantial opportunities for achieving computational efficiency if Eqn. (2) (i.e., the relationships between concentration at the monitoring points c_j ($j = 1, 2, \ldots, M$) and the pumping rates q_i ($i = 1, 2, \ldots, N$) as defined by Eqns (4)–(6) could be mapped approximately using a multivariate function. The key concept that makes it possible is the use of artificial neural networks (ANNs).

An ANN is a nonlinear mathematical structure which is capable of representing arbitrarily complex nonlinear processes that relate the inputs and outputs of any system. Mathematicians have shown that multilayer feed-forward ANNs have the powerful capability to be 'universal function approximators.' Hecht-Hiesen (1990) proved that a three-layer feed forward ANN meets the requirements to be a universal mapping function and that any multivariate function can be approximated by an ANN having only a finite number of nodes in the hidden layer.

The architecture of ANNs is inspired by models of biological neural networks which can recognise patterns and learn from their interactions with the environment. The most widely researched and used structures are multilayer feed-forward networks which are ideally suited for modelling input-output relationships such as the response of the hydraulics and solute transport in the aquifer with respect to the abstraction and injection during remediation.

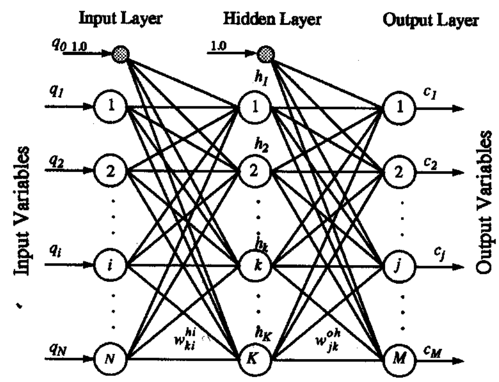


Fig. 1 *The architecture of an ANN*

For the purpose of remediation-scheme designs, an artificial neural network can be considered as a mapping function between an input and an output set. The input set represents the combination of pumping rates in N potential well sites while the output set corresponds the contaminant concentrations at the M monitoring points at the end of the remediation period, with respect to the pumping combinations. The three-layer neural network ANN (N, K, M) is constructed (see Fig. 1) with N neurons in the input layer, K neurons in the hidden layer, and M neurons in the output layer. The network is fully connected between adjacent layers. Each node k receives input from every node i in the previous layer. Associated with each input (q_i) is a weight (w_{ki}^{hi}). The effective input (S_k) to node k is the weighted sum of all the inputs:

$$S_k = \sum_{i=0}^{N} w_{ki}^{hi} q_i \tag{7}$$

where q_0 and w_{k0}^{hi} are called the bias ($q_0 = 1.0$) and the bias weights, respectively. The effective input, S_k, is passed through a nonlinear activation function (sometimes called a transfer function or threshold function) to produce the output (h_k) of the node.

The most commonly-used activation function is the sigmoid function. The characteristics of a sigmoid function are that it is bounded above and below, it is monotonically increasing, and it is continuous and differentiable everywhere. The sigmoid function most often used for ANNs is the logistic function:

$$h_k = f(S_k) = \frac{1}{1 + e^{-S_k}} \qquad k = 1, 2, \ldots, K \tag{8}$$

in which S_k can vary on the range $\pm\infty$, but h_k is bounded between 0 and 1. The output neuron

$$c_j = f\left\{\sum_{k=0}^{K} w_{jk}^{oh} f\left\{\sum_{i=0}^{N} w_{ki}^{hi} q_i\right\}\right\}, j = 1, 2, \ldots, M \quad (9)$$

where w_{ki}^{hi} is a weight between the ith input neuron and the kth hidden neuron, w_{jk}^{oh} is a weight from the kth hidden neuron to the jth output neuron, and f is a sigmoid function as defined by Eqn. (8).

The identification of the structure of the ANN, i.e., the value of K, is usually done using a strategy of progressively adding nodes to the hidden layer until a structure appropriate to the complexity of the problem is achieved, and values for the network weights w_{ki}^{hi} and w_{jk}^{oh} are estimated by means of backpropagation algorithms so that the predicated error is minimised.

Groundwater Remediation Optimization Using GAs

GENETIC ALGORITHMS

Genetic algorithms are a family of combinatorial optimization methods that search for near-optimal solutions of complex problems using an analogy between optimization and natural selection, developed by Holland (1992) and his associates.

The GAs are able to search complex multimodal decision space and can efficiently handle nonconvexities that cause difficulties for traditional optimization methods. As stated by Goldberg (1989), the structure of the genetic algorithms differs from more traditional optimization methods in four major ways: (1) the GA typically uses a coding of the decision-variable set, not single variables themselves; (2) the GA searches within a population of decision-variable sets, not a single decision-variables set; (3) the GA uses the objective function itself, not derivative information; and (4) the GA uses probabilistic, not deterministic, search rules.

The procedures for a simple genetic algorithm can be depicted as in Fig. 2.

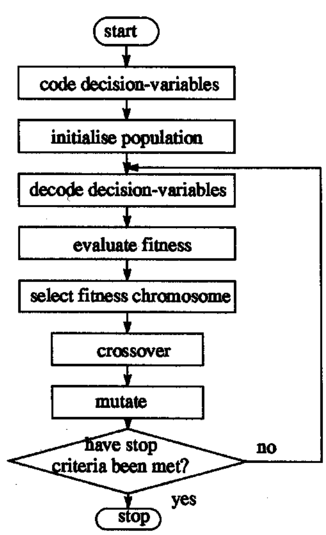


Fig. 2 *A flowchart describing a simple genetic algorithm*

DECODE AND ENCODE DECISION VARIABLES

The genetic algorithm requires that the decision variables describing trial solutions to the pumping realisation be represented by a unique coded string of finite length. This coded string is similar to the structure of a chromosome of the genetic code. On the basis of Goldberg's recommendation, a binary coding was adopted (see Fig. 3). For each potential site, a single bit describes pumping (abstraction/injection) flag, i.e., the values of the variable y_i, and a series of n bits represents the pumping rate at that location. The number of bits n used to represent each pumping rate is a binary resolution and is designed as a GA input parameter. Another two GA input parameters, the minimum and maximum pumping rates per well, are used to decode the binary representations of the pumping rates into real values and which allows the explicit incorporation of the constraint set (3) in the mathematical model. The binary resolution n is chosen, in conjunction with the minimum and maximum pumping rates, so that the desired pumping-rate precision is achieved. The number of genes per string m (the string length) is a function of the number of potential well sites, N and the binary resolution for each well, n, i.e., $m = (n + 1)N$.

According to Eqn. (3), the value of pumping rate for the generated string is decoded as follows:

$$q_i = y_i\left(q_i^{low} + \frac{A_i}{A}(q_i^{up} - q_i^{low})\right) \quad i = 1, 2, \ldots, N$$

where $A = 2^n - 1$ and A_i, $i = 1, 2, \ldots, N$ is the actual decimal value of the corresponding binary substring of the pumping well i.

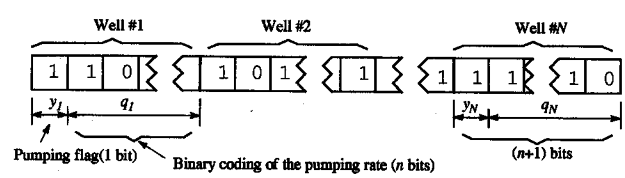


Fig. 3 *String structure for the genetic algorithm formulation*

For example, if there are four potential wells as shown in Figure 4, and each well has a binary substring of three bits, the following 12-gene string might occur: 000101110111. Assuming a maximum pumping rate per well of one unit and a minimum pumping rate of zero, the string, once decoded, represents a well system where well 1(000) is a predefined injection site and has no pumping; well 2(101) is also an injection well but has one third of a unit of pumping; well 3(110), an abstraction well, has two-thirds of a unit of pumping, and the well 4(111), another abstraction well, has one unit of pumping.

PROCEDURES

The procedures of the genetic algorithm employed in this application can be derived as follows:

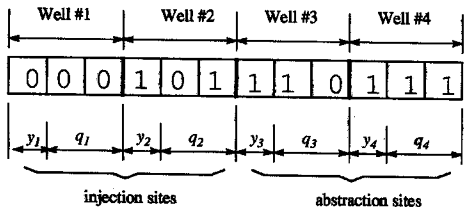


Fig. 4 *An example string for a GA coding and decoding*

Step 1. Generation of initial population.

The GA randomly generates an initial population of coded strings representing realisation of pumping of population size *P* (typically in the range of 100 to 200) as described above.

Step 2. Groundwater flow and contaminant simulation and training of an ANN.

As described previously, the behaviour of complex groundwater scenarios with spatially variable transport parameters and contaminant plume is simulated with a specific simulation model to develop the set of samples upon which the neural network is trained. The input of the ANN characterise the different configurations of pumping wells and their pumping rates. The output is contaminant concentration at the monitoring points at the end of the remediation period.

Step 3. Computation of system cost.

The GA considers each of the *P* strings in the population in turn. It decodes each substring into the corresponding pumping locations and their pumping rates, then computes the total cost of each trial realisation in the current population. The total cost is composed of (1) the capital and operating costs of the pumping configuration according to Eqns (1) and (2), the penalty cost assigned by the GA if there is a violation of the regulatory concentration standard at any monitoring point at the end of the remediation period. The concentration at the monitoring point at which the concentration deficit is maximum is used as the basis for computation of the penalty cost. The maximum deficit is multiplied by a penalty factor λ, which is a measure of the cost for a deficit of one unit concentration.

Step 4. Computation of the fitness.

The fitness of the coded string is taken as some function of the total system cost. The GA computes the fitness for each proposed pumping configuration in the current population as the inverse of the total cost from Step 3.

Step 5. Generation of new population using the selection operator.

The GA generates new members of the next generation by a selection scheme. The selection probability of string *i*, p_i, to go into the next generation of *P* members using proportionate selection methods is given by $f_i / \sum_{j=1}^{N} f_j$ where f_i, is the fitness of string *i* (determined in Step 4).

Step 6. The crossover operation.

Crossover is the partial exchange of bits between two parent strings to form two offspring strings. Crossover occurs with some specified probability of crossover p_c for each pair of parent strings selected in Step 5. To perform one-point crossovers, a crossover point is randomly selected along the strings. The crossover operator exchanges the bits after the crossover point between the two selected parent strings.

Step 7. The mutation operation.

Mutation occurs with some specified probability p_m for each bit in the strings which have undergone crossover. The bitwise mutation operator changes the value of the bit to the opposite value (i.e., 0 to 1 or 1 to 0).

Step 8. Production of successive generations.

The use of the three operators described above produces a new generation of pumping realisation using Steps 2 to 7. The GA repeats the process to generate successive generations. The least cost strings (e.g., the best 5) are stored and updated as cheaper cost alternatives are generated. Typically, a GA will evaluate between 100 and 1000 generations.

Application Example

AQUIFER DESCRIPTION

The model described has been used to design a pump-and-treat remediation scheme for a simplified approximation of a real aquifer contaminated with chlorinated solvents. For the purpose of this exercise, the aquifer is assumed to be confined, homogeneous and isotropic with dimensions of 500 by 500 metres as shown in Fig. 5. This aquifer is modelled using a uniformly-spaced grid consisting of 51 by 51 nodes, 2500 finite-difference grid evenly spaced at 10-metre interval. In the model runs, the solutions were constrained to meet a regulatory contaminant concentration of 20 *ppb* in the effluent from the treatment facility and in the aquifer at the end of remediation. Abstraction and injection rates were constrained between a minimum of 0 and a maximum of 2.0 ls^{-1}. The remediation time period was assumed to be 20 years with a discount rate of 10 percent. In the model runs, 16 wells were available for pumping and 25 nodes were used as compliance points. The aquifer properties used in the model are listed in Table 1.

The goal of remediation is to keep the contaminant-mass concentrations from moving off site, i.e., past the line of monitor wells in amounts that are above the regulatory concentration limit. The measure of remediation efficiency (i.e., objective function) is to minimise the total cost of installation, pumping (abstraction and injection) and treat-

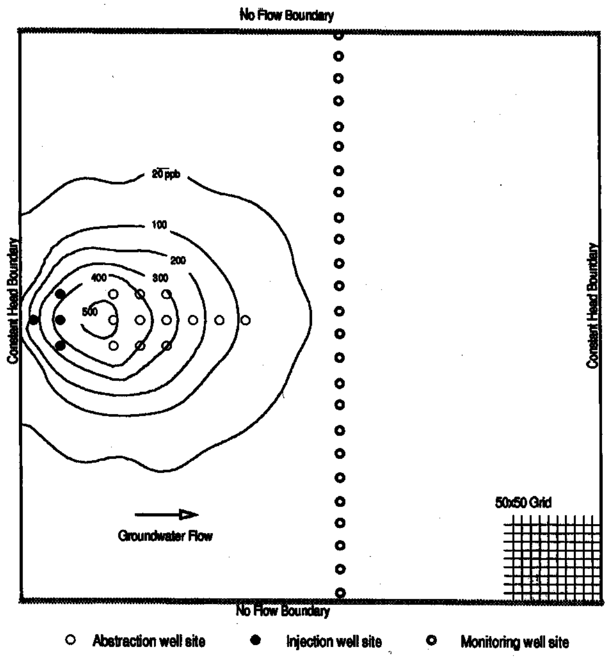


Fig. 5 *Groundwater remediation problem schematic*

Table 1. Aquifer and contaminant transport parameter values

Parameter	Value
Hydraulic conductivity (K)	6.0×10^{-6} m/s
Longitudinal dispersivity(ε_L)	25 m
Transverse dispersivity(ε_T)	2.5 m
Porosity (ϕ)	0.2
Diffusion coefficient (D_d)	2.6×10^{-9} m^2/s
Saturated thickness (b)	50 m
Time step for mass transport (Δt)	7.884×10^6s
Number of time steps	80
Density of soil	2.69 g/cm^3
Bulk density of aquifer material	2.23 g/cm^3

ment. It is assumed that the pumping rates will be kept constant during the remediation period.

DEVELOPMENT OF TRAINING AND TESTING PATTERNS

A 2-Dimensional hybrid finite-difference/finite-element flow and transport code, FDMOD, was used to simulate numerically the effects of different pumping patterns, thereby establishing a knowledge base for training and testing the neural networks. The patterns represented not only a random sample from the domain of possible subsets for all potential locations but also patterns thought to reflect important boundary conditions and good pumping strategies from a hydrological standpoint. The results from these simulations provided the estimates of the contaminant concentrations at the monitoring point at the end of the remediation period with respect to the various pumping configurations. Utilising a neural network in place of the simulation model during the optimization phase reduces the computational burden by more than two orders of magnitude.

To achieve best results, the orthogonal array method (Taguchi, 1987) was adopted to design the simulation experiments. For each simulation run, the pumping rate for each well (abstraction or injection) takes one of three values (1, 2 or 3) corresponding to non-pumping, half-maximum and full-maximum pumping respectively.

Three training and testing pattern sets containing a total of 500 pumping configurations were developed. The sets were not homogenised in order to ascertain whether certain methods for generating training sets had advantages over others. The first set of 300 was formulated using a randomly-generated orthogonal array. The second set of 50 was created using hydrogeological insight to choose likely pumping regimes and variations thereof. The third set was contrived by adding/deleting pumping wells to examples of high-ranking pumping realisations from the first two sets. Although a two-dimensional model has been used here for illustration purposes, a three-dimension model could have been used just as easily.

TRAINING OF NEURAL NETWORKS

The type of neural network used in this study was chosen as a three-layer, feed-forward perceptron trained with the use of a back-propagation learning algorithm. The initial approach was to have the input vector represent a possible configuration of the pumping wells. As 16 possible pumping wells were being considered, each input was a row vector of 16 variables; a variable value of 1 indicates that the well was chosen as a pumping well with full maximum pumping rate and 0 indicated it was not selected. The output vector comprises 25 variables corresponding to the contaminant concentration at the monitoring points at the end of the remediation period. The number of the hidden nodes was identified using the strategy of progressively adding nodes to the hidden layer until the best result is achieved. The appropriate structure for this example was ANN(16, 8, 25).

During the course of training, 400 out of the 500 patterns developed were used to train the neural network and the remaining 100 patterns which were not involved in the training were used to test the neural network. The performance accuracy of the trained network was 100% for the first test pattern set and the generalisation performances were 88% and 93% for the test pattern sets 2 and 3 respectively.

SEARCH FOR OPTIMAL PUMPING PATTERNS

Once the network has been trained to a predefined level of performance, it can be used to examine as many combinatorial possibilities as desired. Theoretically, all possibilities could be examined to ensure a global minimum but obviously that is impossible in practice. Therefore, a genetic algorithm was employed to search for optimal pumping patterns. An initial population of 200 successful patterns evolved through 300 generations according to a simple three-generator genetic algorithm to produce some 60, 000 pumping patterns (see Table 2 for parameters). Finally, three highest-ranking pumping patterns were selected as the most successful remediation schemes for the aquifer under study as listed in Table 3.

Table 2. Input parameter set for the GA

Parameter	Value
Binary resolution per well	8 (plus one for abstraction/injection)
Population size	200
Number of genes per string	144
Generations	300
Mutation probability	0.04
Crossover probability	0.85
Selection ratio	0.90

CONFIRMATION OF REMEDIATION SCHEMES

The recommended pumping configurations were confirmed as successful with the aid of the groundwater flow and transport simulation model. If no remediation were undertaken, plots of the concentration contours over time (Fig. 6) indicated initial contaminant concentrations approaching the monitoring-well line exceed 100 *ppb*. Similar plots produced following the implementation of the recommended optimal design showed no concentrations above 20 *ppb* reaching the monitoring wells (Fig. 7) at the end of the 20-year remediation period.

Conclusion and Discussion

An optimization model based on a hybrid neural network/genetic algorithm was used to investigate the minimum-cost design of a pump-and-treat aquifer remediation scheme. This mixed-integer nonlinear approach has been devised to find the least-cost solution for both pumping and treatment components which include the fixed costs of construction and the variable costs associated with operation/maintenance. To that end, an artificial neural network is trained to predict the performance of a particular configuration of the abstraction and injection wells and their possible pumping rates combinations. After the network has been suitably trained, the GA searches through possible combinations of the pumping wells, using the trained neural network to predict the performance and subsequently the merit rating of each configuration.

This hybrid algorithm has several advantages. Firstly, the algorithm involves less computational burden and more flexibility. In this approach, the groundwater flow and contaminant simulations, usually the time-consuming components, are not coupled with the optimization scheme as subroutines as they should be in conventional optimization techniques but are used to establish a knowledge base for training the neural network. Moreover, the increased flexibility provided by parallel processing of the simulations and 'recycling' of the simulation, results in the

Table 3. Three recommended remediation schemes

Scheme No.	Nodes	Pumping rate (l/s)		Normalised total cost
		Injection	Abstraction	
1	(4, 25)	2.00		1.00
	(11, 25)		1.68	
	(14, 25)		1.68	
	(17, 25)		1.04	
2	(1, 25)	1.28		1.036
	(4, 25)	2.00		
	(11, 25)		2.00	
	(17, 25)		1.68	
3	(4, 25)	2.00		1.053
	(11, 25)		2.00	
	(17, 22)		1.68	
	(17, 28)		1.68	

Fig. 6 *Concentration contours over time—Without remediation*

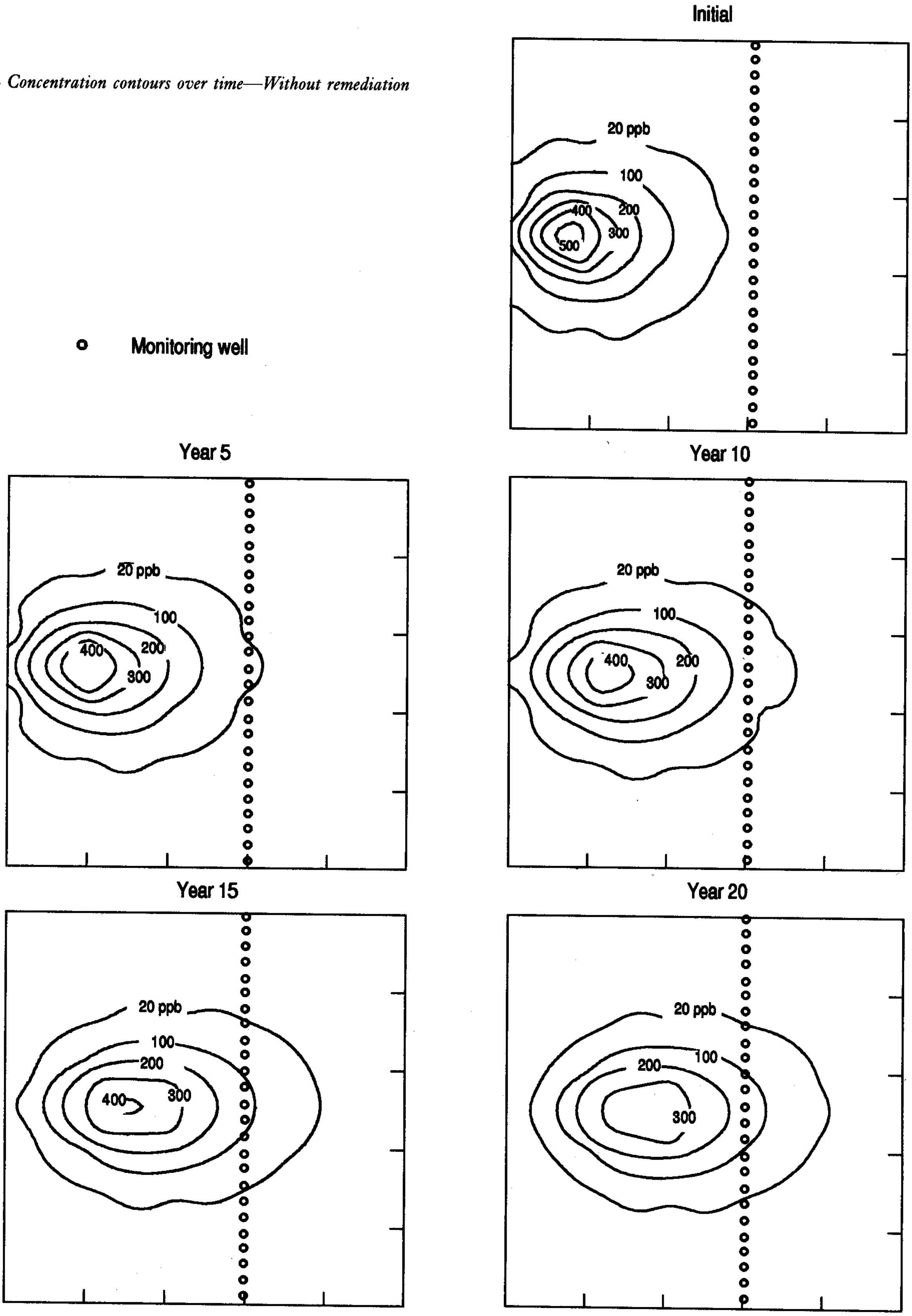
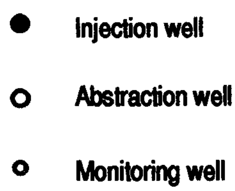
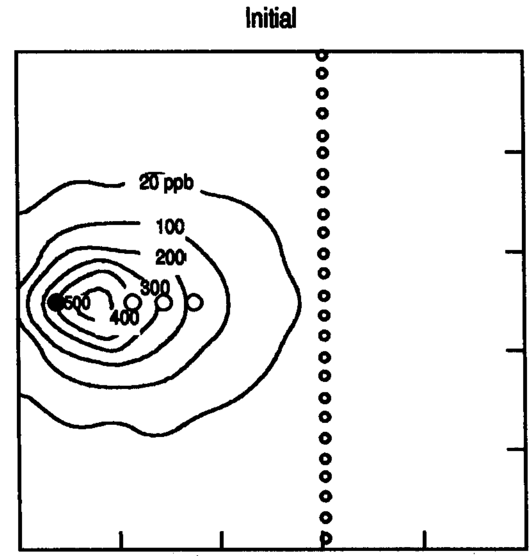
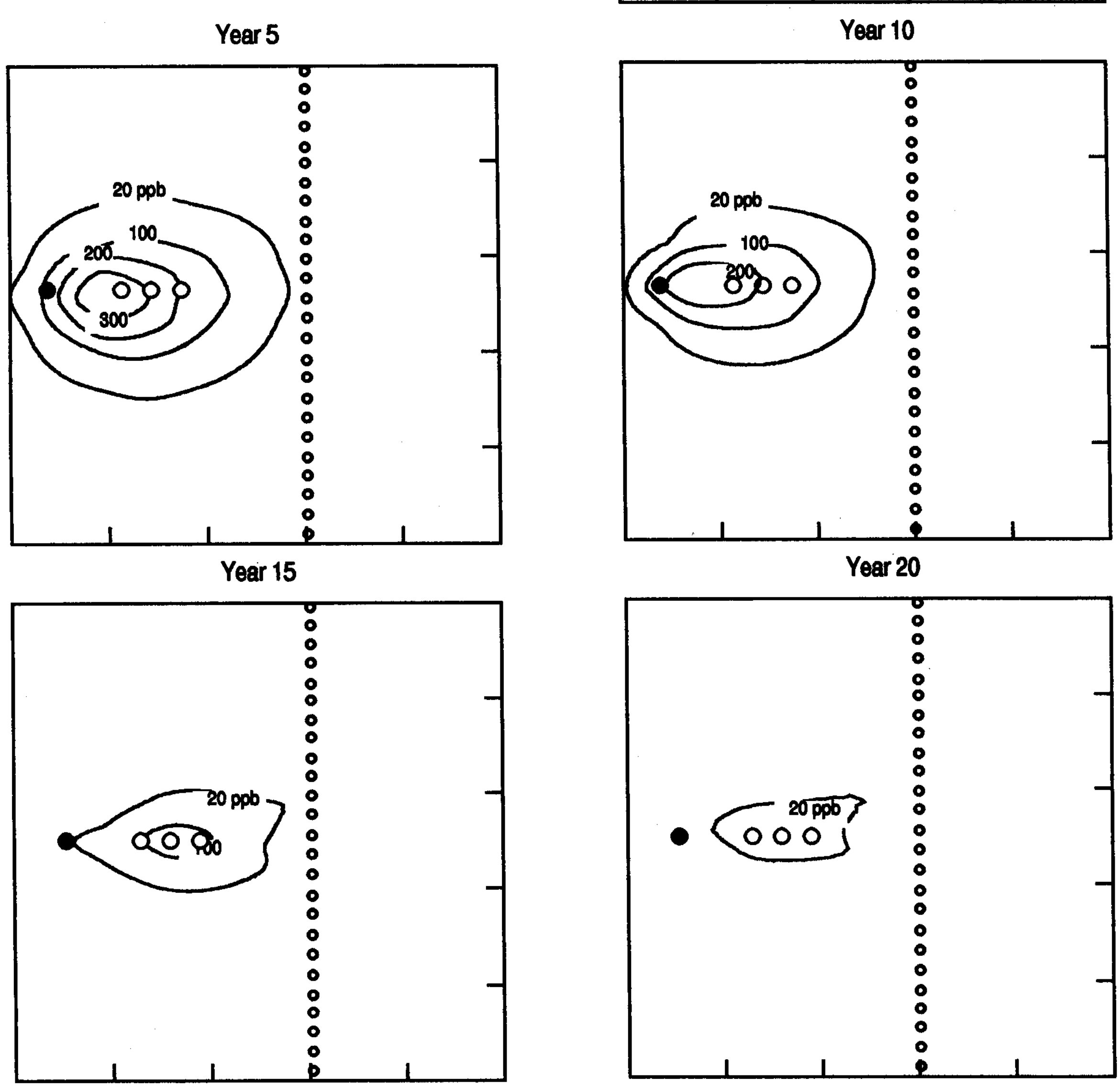


Fig. 7 *Concentration contours over time—Optimal remediation scheme*







reduction of computational burden which is usually an obstacle to field-scale applications. In addition, the algorithm provides more independence from the simulation model structures and simulation methods. This independence has the subsequent advantage of incorporating any appropriate groundwater flow and solute transport simulation code, ranging from 1 to 3-dimensional, according to the specific site conditions and data availability, etc.

The algorithm has been shown to be effective in a series of simplified but representative problems. Based upon the preliminary results presented here, it is expected that the proposed methodology will behave similarly in large-scale, real-world applications. Therefore, this methodology is to be made available through WaterWare (Jamieson and Fedra, 1996), a comprehensive decision-support system for river-basin planning. In the fullness of time, other groundwater remediation processes, such as engineering barriers, in-situ treatment, etc., will be included, recognising that the pump-and-treat methodology may not be the most appropriate in all circumstances.

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