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Optimal Management of Coastal Aquifers Using Linked Simulation Optimization Approach

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Abstract. Saltwater intrusion management models can be used to derive optimal and efficient management strategies for controlling saltwater intrusion in coastal aquifers. To obtain physically meaningful optimal management strategies, the physical processes involved need to be simulated while deriving the management strategies. The flow and transport processes involved in coastal aquifers are difficult to simulate especially when the density-dependent flow and transport processes need to be modeled. Incorporation of this simulation model within an optimization-based management model is very complex and difficult. However, as an alternative, it is possible to link a simulation model externally with an optimization-based management model. The GA-based optimization approach is especially suitable for externally linking the numerical simulation model within the optimization model. Further efficiency in computational procedure can be achieved for such a linked model, if the simulation process can be simplified by approximation, as very large number of iterations between the optimization and simulation model is generally necessary to evolve an optimal management strategy. A possible approach for approximating the simulation model is to use a trained Artificial Neural Network (ANN) as the approximate simulator. Therefore, an ANN model is trained as an approximator of the three dimensional density-dependent flow and transport processes in a coastal aquifer. A linked simulation – optimization model is then developed to link the trained ANN with the GA-based optimization model for solving saltwater management problems. The performance of the developed optimization model is evaluated using an illustrative study area. The evaluation results show the potential applicability of the developed methodology using a GA- and ANN-based linked optimization – simulation model for optimal management of coastal aquifer.

Key words: artificial neural networks, coastal aquifers, genetic algorithms, groundwater, management, optimization, saltwater intrusion

1. Introduction

Unplanned exploitation of water from coastal aquifers hydraulically connected with sea or ocean may cause saltwater intrusion in coastal aquifers. Therefore, the exploitation of coastal aquifers is often restricted due to excessive saltwater intrusion. Efficient management strategies are needed for optimal withdrawal of water from coastal aquifers, while maintaining salt concentration under specified permissible limit.

The physical processes involved in a coastal aquifer are needed to be simulated accurately, to obtain physically meaningful optimal management strategies. Therefore, a saltwater intrusion simulation model needs to be incorporated within the management model, so as to ensure feasibility of the obtained optimal strategies. The simulation of the flow and transport processes involved in coastal aquifers is difficult as the density-dependent flow and transport processes need to be modeled. Incorporation of this simulation model within an optimization-based management model is complex and difficult. Embedding technique and response matrix approach (Gorelick, 1983) are the two methods generally used to incorporate the simulation model within the management model. Embedded optimization models use finite difference or finite element approximation of flow and transport equations as equality constraints within the management model, along with other physical and managerial constraints. The use of embedding technique for saltwater intrusion management model (Wills and Finney, 1988; Das and Datta 1999a,b) has several limitations for large-scale aquifer systems. This approach is also numerically inefficient when applied to large aquifer systems with considerable heterogeneity. The response matrix approach is based on the principle of superposition and linearity. This method is reported to be unsatisfactory for highly nonlinear systems (Rosenwald and Green, 1974). As an alternative to these methods, a linked simulation – optimization (Gorelick, 1983; Emch and Yeh, 1998) approach may be useful to solve the saltwater intrusion management model. The performance of the linked simulation – optimization approach is highly dependent on the performance of the saltwater intrusion simulation model, as repetitive simulations are required to achieve an optimal management strategy. Simulation of density-dependent saltwater intrusion process in coastal aquifer is complex and costly in terms of computational time and computer memory requirements. Incorporation of a highly nonlinear simulation model within the management model would take considerably large computational time to achieve any optimal solution. The computational time requirement can be reduced through parallel computing, or by some approximation of the simulation model. The former approach may be more accurate as a more rigorous numerical model is used, but will be more costly in terms of computer hardware requirement, as it needs parallel computing facilities. The later approach involves the approximation of the original simulation model. This approach will be less costly in terms of computational time and computer hardware requirements. A possible alternative is to use a trained ANN model as an approximate simulator of the physical processes.

The heuristic search technique, Genetic Algorithm (GA) may be used as a tool for solving the optimum management model, because of its relative efficiency in identifying global optimal solutions especially for nonlinear non-convex problems. The GA-based optimization approach is especially suitable for externally linking the numerical simulation model within the optimization model. This trained (Artificial Neural Network) ANN linked to a GA-based optimization model can be useful in evolving management strategies for coastal aquifers. Therefore, an ANN model is developed to approximate the complex flow and transport processes in coastal aquifers. The performance of the developed ANN model as a simulator of salt intrusion process in coastal aquifer is evaluated using an illustrative study area. A linked simulation – optimization model is then formulated by externally linking the trained ANN with the GA-based optimization model to obtain optimal management strategies.

The flow and transport processes are complex and highly nonlinear in case of coastal aquifers, where both flow and transport processes are density dependent. A transition zone of varying density exists between saltwater and freshwater. Most of the earlier researchers have ignored the transition zone, and assumed that a discrete interface (sharp interface) exists between saltwater and freshwater. The analytical solutions for sharp interface condition were presented by Henry (1959), Bear and Dagan (1964), Hantush (1968), and Strack (1976). Numerical solutions for sharp interface approximation were also presented by Shamir and Dagan (1971), Pinder and Page (1977), Mercer *et al.* (1980), Liu *et al.* (1981), and Taigbenu *et al.* (1984). The sharp interface assumption will be valid, or may give expectable results, if the transition zone is narrow. For large transition zone, sharp interface approximation of the transition zone would result in erroneous results. The numerical simulation of the density-dependent flow and transport processes were presented by Huyakorn *et al.* (1987), Puti and Paniconi (1995), and Cheng and Chen (2001). Das and Datta (2000) presented an optimization-based simulation model of density-dependent saltwater intrusion process in coastal aquifers. They solved finite difference approximation of the density-dependent flow and transport equations simultaneously, without iterating between the two. Essink (2001) modeled saltwater intrusion in a three-dimensional large-scale coastal aquifer in Holland. They utilized a computer code MOCDENS-3D to model the displacement of fresh, brackish, and saline groundwater in the hydrogeolocal system. Simpson and Clement (2003) observed that the standard Henry's problem is largely influenced by the boundary forcing, and not due to the density-dependent effect. Therefore, they have modified the standard Henry's problem by decreasing the freshwater recharge. They compared the numerical results for the modified Henry's problem against semi-analytical results. All these saltwater intrusion simulation models are computationally intensive. Therefore, an approximate solution of the flow and transport processes in coastal aquifer may be useful, if it is sufficiently accurate and computationally less intensive.

An approximate simulation of the flow and transport processes may be useful for linking with an optimization-based management model. Regression analysis and ANN are generally used to approximate flow and transport processes in groundwater. Alley (1986) developed regression equations to relate variation in pumping and recharge rates at five decisions wells to the concentration at nine control locations for two dimensional transport processes in an aquifer. Lefkoff and Gorelick (1990) presented multiple linear regression equations to approximate transport process in an aquifer. This approximation model predicts the change of ground-water salinity resulting from the hydrologic conditions and water-use decisions. Rogers and

Dowla (1994) incorporated ANN with an optimization model to predict total solute mass removal for treatment. They trained an ANN model to predict whether the given set of pumping satisfies the containment constraints. Ejaz and Peralta (1985) also presented regression equations to predict downstream concentration of several constituents from the upstream flow rate and constituent concentration. Morshed and Kaluarachchi (1998) presented an ANN model to approximate concentration break-through curves for one-dimensional unsaturated flow and transport. Aly and Parelta (1999a) trained an ANN to model the response surface within an optimization model. They applied their model to design pump-and-treat systems for aquifer cleanup. Johnson and Rogers (2000) evaluated the effect of using ANN and linear approximator in conjunction with simulated annealing driven search for two different two-dimensional ground-water remediation problems. All these studies were confined to one or two dimensional flow and transport processes.

Classical optimization techniques, e.g. linear programming, nonlinear programming, mixed integer programming, are extensively used for ground-water management models. The main disadvantage of these classical methods is that most of these methods are based on gradient search techniques. Most of the time, these gradients are calculated numerically. The numerical estimation of gradient is the most expensive part of an optimization-based management models. Moreover, numerical calculation of gradients may sometime lead to large errors. Another disadvantage of these gradient search methods is that often it obtains only local optimal solutions, especially when the response surface is highly irregular. The other limitations of classical methods are point-to-point search, necessity of initial guesses, deterministic transition rule, assumption of unimodality, etc. (Deb, 2001). Nowadays, many non-gradient based search techniques have been developed. These are GA, Simulated Annealing (SA), etc. Many researches have used these algorithms for solving optimization-based groundwater management models.

Genetic Algorithms are considered as more powerful and robust tools for function optimization. These algorithms are computationally simple, but powerful in their search for improvement after each generation (Goldberg, 2000). GA mimics some of the processes observed in natural evolution, such as natural selection, etc. (Holland, 1975). The basic techniques of GA are designed to simulate the mechanism of population genetics and natural rules of survival in pursuit of the ideas of adaptation. One of the great advantages of GA is that it does not require differentiability of either the objective function or the constraint function. GA does not assume unimodality of the objective function. The constraints handling capacity of GA are also better than that of classical optimization techniques, because of the population-based approach in GA (Deb, 2001).

Ritzel *et al.* (1994) applied GA to solve a two objectives steady state groundwater pollution contaminant problem. The two objectives were: maximize reliability and minimize cost of the hydraulic containment system. Mckinney and Lin (1994) used GA for single objective groundwater management problems. They solved three example problems. The first example problem determines the maximum yield from a homogeneous isotropic unconfined aquifer system. In the second example problem, they determined minimum cost combination of wells to supply an exogenous demand of water from an unconfined aquifer system. The objective of the third example problem was to minimize the cost required for pump-and-treat remediation system design to remove a contaminant from an aquifer, using air stripping technology. Rogers and Dowla (1994) presented an optimization model for groundwater remediation using artificial neural networks and GA. They applied artificial neural networks to predict the outcome of the flow and transport simulation. Cieniawski *et al.* (1995) used GA to solve a multi-objective groundwater monitoring problem. The two objectives were: maximize reliability, and minimize contaminated area at the time of first contamination detection. Aly and Peralta (1999a) presented a methodology for optimal design of aquifer cleanup systems under uncertainty using neural networks and GA. Again in the same year, Aly and Peralta (1999b) presented a comparison between GA and mathematical programming for the design of groundwater cleanup system for several optimization scenarios. Morshed and Kaluarachchi (2000) reviewed the application of GA in solving groundwater optimization problems. More recently, Aral *et al.* (2002) combined groundwater simulation model with GA for identification of contaminant source locations and release history in aquifers.

The proposed methodology uses a trained ANN as an approximate simulator of the three-dimensional density-dependent flow and transport processes in a coastal aquifer. The trained ANN is linked to a GA-based optimization model. An embedded optimization-based simulation model (Das and Datta, 2000) is used to generate required patterns for training and testing of the multi-layered perceptron (ANN). The ANN model is linked as an external module to the optimization model. The objective of the management model is to maximize optimal extraction of water withdrawal for beneficial use from the coastal aquifers, while maintaining salt concentration of the pumped water under specified permissible limits. Real coded genetic algorithm is used to solve the optimization-based management model. The performance of the developed simulation – optimization (ANN–GA) model is evaluated using an illustrative study area.

2. Simulation Model

In the present study, an optimization-based simulation model (Das and Datta, 2000) is used to generate required patterns for training and testing of the ANN model. Density-dependent saltwater intrusion process in a coastal aquifer is simulated by simultaneously solving the governing equations for three-dimensional advective-dispersion flow and transport processes. The three-dimensional advective-dispersive flow equation may be written as (Huyakorn *et al.*, 1987):

$$\frac{\partial}{\partial x_i}\left[K_{ij}\left(\frac{\partial h}{\partial x_j}+\eta c e_j\right)\right)=S_S\frac{\partial h}{\partial t}+\phi\eta\frac{\partial c}{\partial t}-\frac{\rho}{\rho_o}q \tag{1}$$

where, K_{ij} is the hydraulic conductivity tensor, h is the reference hydraulic head, η is the density-coupling coefficient, c is the dimensionless solute concentration ($0 \leq c \leq 1$), e_j is the jth component of gravitational unit vector, S_S is the specific storage, t is time, ϕ is the porosity, q is volumetric flow rate of sources or sinks per unit volume of the porous medium, ρ and ρ_o are the density of mixed fluid and reference density, respectively.

The reference hydraulic head is defined as

$$h = \frac{p}{\rho_0 g} + Y \tag{2}$$

where, p is the fluid pressure, g is the gravitational acceleration, and Y is the elevation above datum.

The density coupling coefficient is defined as

$$\eta = \frac{\varepsilon}{c_S} \tag{3}$$

where, ε is density difference ratio expressed as,

$$\varepsilon = \left(\frac{\rho_S - \rho_o}{\rho_o}\right) \tag{4}$$

and, c_S is the solute concentration corresponding to the maximum density ρ_S. The actual hydraulic conductivity is defined as

$$K_{ij} = \frac{k_{ij}\rho g}{\mu} \tag{5}$$

Where, k is the intrinsic permeability tensor (L^2), μ is the dynamic viscosity of fluid and μ_o is the viscosity of the freshwater.

The density of the mixed fluid is defined as

$$\rho = \rho_o\left(1 + \varepsilon\frac{c}{c_S}\right) \tag{6}$$

The advective-dispersive equation can be written as

$$\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial c}{\partial x_j}\right) - V_i\frac{\partial c}{\partial x_i} = \phi\frac{\partial c}{\partial t} + qc \tag{7}$$

Where, $D_{ij} = \phi\tilde{D}_{ij}$, with $\tilde{D}_{ij}$ is the dispersion tensor and V_i is the Darcy velocity vector. The Darcy velocity vector is expressed as

$$V_i = -K_{ij}^o\left[\frac{\partial h}{\partial x_j} + \eta c e_j\right] \tag{8}$$

where, K_{ij}^o is the hydraulic conductivity at the reference condition.

The flow Equation (1) and transport Equation (7) are coupled *via* density coupling term and Darcy's velocity. This coupling between the flow and transport equation make the saltwater intrusion process highly nonlinear. To simulate the flow and transport processes, the flow and transport equations are discretized using finite difference technique. The set of discretized equations are then solved using nonlinear optimization system, MINOS (Murtagh and Saunders, 1993) for specified initial and boundary conditions. A detailed description of the simulation procedure using the optimization-based simulation model to solve flow and transport equations is available in Das and Datta (2000).

3. Development of ANN Model

The universal approximator, Artificial Neural Networks, mimics the function of human brain by acquiring knowledge through process of learning. The learning process involves finding of an optimal set of weights for the synaptic connections between artificial neurons of the network. The ability to gather knowledge through the process of learning, like a human brain, from sufficient predictor patterns makes it possible to apply the ANN to solve large-scale real world problems. Once the ANN is trained, the relationship between the predictor (input) and predicted (output) variables is encoded in the network. Then it can be used to predict the output based on the information fed to the input nodes.

The predictive efficiency of an ANN model is largely dependent on the architecture of the ANN model. The present study adopts a single hidden layer standard back-propagation feed-forward ANN model. This model has three neuron layers. These are the input, output, and hidden layers. The number of neurons in the input layer are equal to the number of input parameters. The number of neurons in the output layer are equal to the number of output parameters. The number neurons in the hidden layer are dependent on the complexity and nonlinearity of the problem. A unipolar sigmoidal function is used as the transfer function. The sigmoidal function is expressed as:

$$f(\boldsymbol{x}) = \frac{1}{1 + e^{-x}} \tag{9}$$

A study was conducted to relate the number of neurons in the hidden layer, with the best values of learning rate and momentum rate. The best value of learning rate and momentum rate are judged on the basis of average relative error (RE) and average coefficient of correlation (R^2). Relative error and coefficient of correlation may be defined as follows:

$$\mathrm{RE} = \frac{1}{N} \sum_{n=1}^{N} \left(\left| \frac{C_n' - C_n}{C_n'} \right| \right) \tag{10}$$

and,

$$R^2 = \frac{\frac{1}{N}\sum_1^N (C'_n - \overline{C'})(C_n - \overline{C})}{\sqrt{\frac{(C'_n - \overline{C'})}{N}}\sqrt{\frac{(C_n - \overline{C})}{N}}} \tag{11}$$

Where, C'_n is the observed saltwater concentration, C_n is the predicted saltwater concentration, $\overline{C'}$ is the mean of observed concentration, $\overline{C}$ is the mean of predicted concentration, and N is the sample size. On the basis of trial and error evaluation of the ANN architectures, the number of neurons in the hidden layer is taken as number of neurons in the input layers. A constant learning rate of 0.08, and a constant momentum rate of 0.65 are used in this study. The most commonly used algorithm, back propagation, is used to train the networks. This algorithm first computes the error signal at the output layer, and then it is propagated to the input layer through hidden layer(s). After computing error signals, this algorithm will first adjust the synaptic weights between hidden and output layers, and only then adjust the synaptic weights between input and hidden layers. These procedures will continue till the error between target output and the model output is less than the specified permissible value. A C-program is developed to implement the back propagation algorithms.

An optimization-based simulation model (Das and Datta, 2000) is used to generate training and testing patterns for the ANN model. The input to the ANN model is the set of transient pumping rates, generated using a uniform distribution for specified upper and lower limits. The set of transient pumping values are then used as input to the optimization-based simulation model for transient simulation. The resulting salt concentrations of the pumped water at different time steps are specified as output patterns. The ANN is trained by back-propagation algorithm. Once the ANN is trained, outputs from the ANN model are the salt concentrations of the pumped water at different time steps. In the illustrative example, we have taken eight pumping wells, and simulation is carried over a period of one and half year. Each time step is of 6 months. Therefore, number of input and output of the ANN model is equal to 24. The relationship between input and output may be expressed as:

$$\left(C_i^t, i = 1, \ldots, 8; t = 1, \ldots, 3\right) = f\left(P_i^t, i = 1, \ldots, 8; t = 1, \ldots, 3\right) \tag{12}$$

Here, i is the index for pumping location, and j is the index for time step; C_i^j is the salt concentration from pumped water at pumping well, at time step t; P_i^t is the pumping from the pumping well i, at time step t.

The total set of generated patterns has been divided into three subsets. About 200 patterns are kept aside for validation, 200 patterns for prediction, and the remaining 2000 are used for training the neural network. The training pattern will determine the synaptic weights of the networks during training phase. The validation error is carefully monitored during the training phase, and the training is just stopped before the validation error starts increasing. Therefore, validation set will determine the stopping criteria for training. The prediction set will determine the performance of the ANN on a new dataset.

4. Development of Management Model

A saltwater intrusion management model is formulated using the linked simulation – optimization approach to evolve an optimal management strategy. The objective of the optimization model is to maximize total withdrawal of water from a coastal aquifer while maintaining salt concentration of pumped water under specified permissible limit. The water is pumped from preselected pumping locations, and it is assumed that strainers are located in a particular layer at a given pumping location. It is also assumed that the pumping from a well is constant for a period equal to the specified time step. The general formulation of the transient-saltwater management model may be mathematically represented as follows.

$$\text{Maximize} \quad \sum_{t=1}^{T} \sum_{n=1}^{N_\mathrm{w}} Q_n^t \tag{13}$$

$$\text{Subjected to} \quad \boldsymbol{C} = f(\boldsymbol{Q}) \tag{14}$$

$$C_n^t \leq C(u)_n^t \quad n = 1, \ldots, N_\mathrm{w}; t = 1, \ldots, T \tag{15}$$

$$Q(l)_n^t \leq Q_n^t \quad n = 1, \ldots, N_\mathrm{w}; t = 1, \ldots, T \tag{16}$$

$$Q_n^t \leq Q(u)_n^t \quad n = 1, \ldots, N_\mathrm{w}; t = 1, \ldots, T \tag{17}$$

Here, Q_n^t is the pumping from the nth well at time step t; T is the total time steps; N_w is the total number of wells; $\boldsymbol{C}$ represents a vector of simulated salt concentrations as obtained from solution of the simulated model; $\boldsymbol{Q}$ is a vector of spatial and temporal pumping rates from specified potential pumping locations; C_n^t is the salt concentration of the pumped water at nth well at time step t; $C(u)_n^t$ is the upper limit of salt concentration of the pumped water at nth well at time step t; $Q(u)_n^t$ is the upper limit of pumped water from the nth well at time step t; $Q(l)_n^t$ is the lower limit of pumped water from the nth well at time step t.

The objective function (13) along with the constraints (14) to (17) constitute a nonlinear optimization problem. The salt concentrations of the pumped water are simulated using the developed ANN model. The ANN model is externally linked with the optimization model. The pumping information from the optimization model is sent to the ANN model. The ANN model simulates salt concentrations of the pumped water, and sends this information back to the optimization model. Figure 1 shows a schematic representation of the developed methodology using a linked simulation – optimization model.

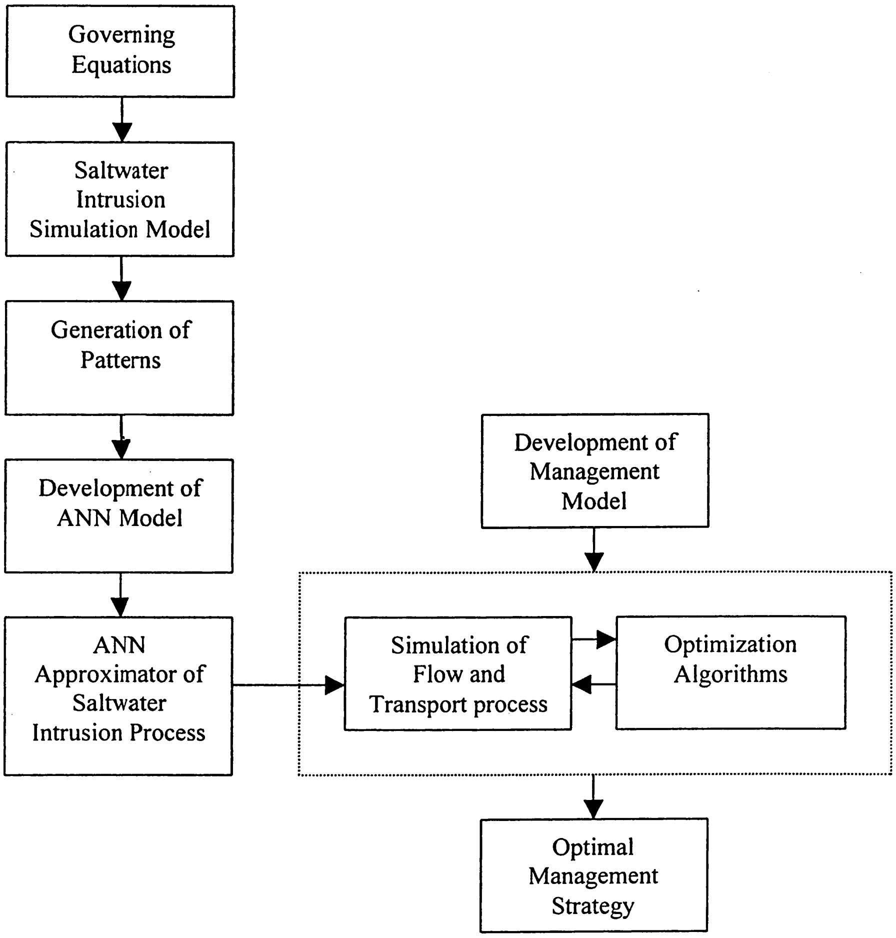


Figure 1. Schematic representation of the simulation-optimization approach.

5. Illustrative Study Area

The performance of the developed ANN model is evaluated by applying the simulation – optimization model to an illustrative study area as shown in the Figure 2. The area of the aquifers is 2.52 km^2 (1.8 (length) $\times$ 1.4 (width)) and the thickness of the aquifer is 100 m. The confined aquifer system is subjected to saltwater intrusion along the coastal side of the study area. The right-hand face of the aquifer is the ocean face, which allows the saltwater to enter in to the aquifers through the bottom of the aquifers, and also allows the exit of the mixed water from the top of the aquifers. It is assumed that mixed water can exit the aquifer through the top 20% of the aquifer, at the ocean face. The left-hand side of the aquifers is inland face, which allows fresh water to enter the aquifers. Top of the aquifer is

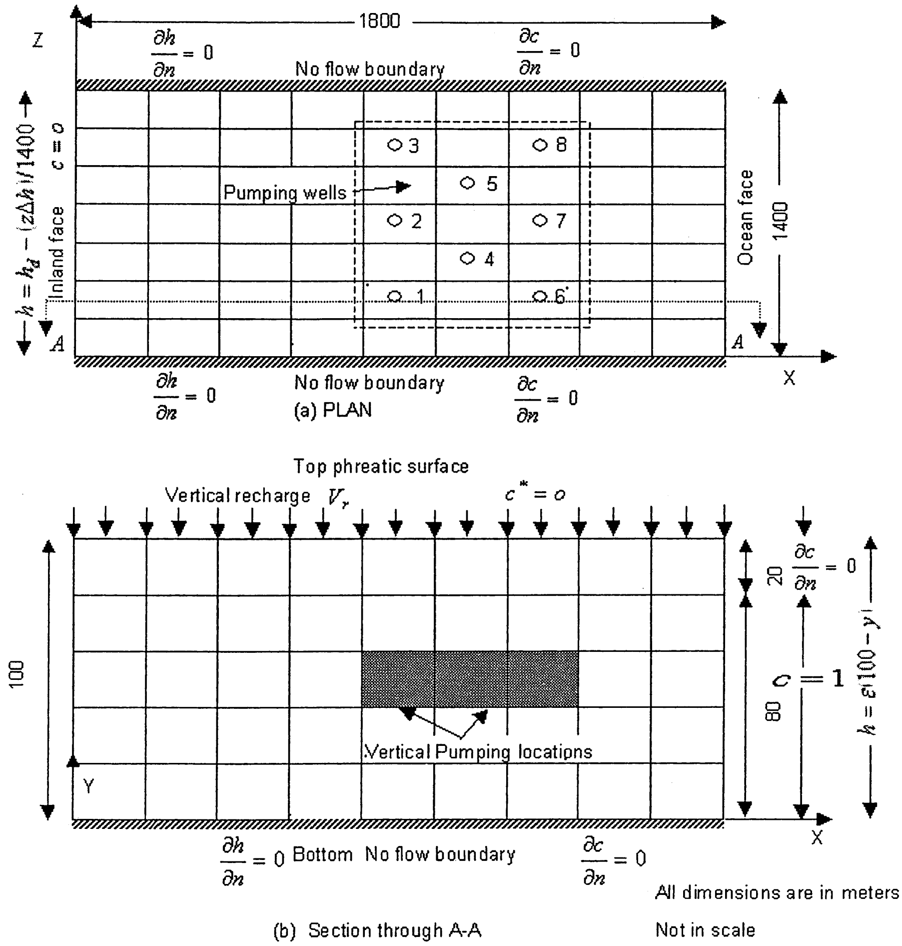


Figure 2. Illustrative study area.

considered as phreatic. Uniformly distributed vertical discharges occur though the phreatic surface. The other three faces, front, back, and the bottom of the aquifer are considered as impermeable. The three-dimensional confined hypothetical aquifer is assumed to be homogeneous and anisotropic, with respect to fresh water hydraulic conductivity, molecular diffusion, and longitudinal and transverse dispersivities. The aquifer parameters values are specified in Table I.

The boundary condition in the aquifer (Figure 2) is considered as time invariant. The flow boundary condition on the ocean face is considered as hydrostatic in vertical direction (Huyakorn *et al.*, 1987; Das and Datta, 2000). This may be written as:

$$h = \varepsilon(100 - y) \tag{18}$$

Table I. Values of aquifer parameters

Hydraulic conductivity in x direction K^o_{xx}, m/day	25.00
Hydraulic conductivity in y direction K^o_{yy}, m/day	0.25
Hydraulic conductivity in z direction K^o_{zz}, m/day	25.00
Longitudinal dispersivity α_l, m	80.00
Lateral dispersivity α_t, m	25.00
Molecular diffusion d_o, m/day	0.69
Density difference ratio ε	0.025
Soil porosity ϕ	0.28
Vertical recharge V_r, m/year	0.02

where, ε is the density difference ratio, and y is the vertical distance from bottom of the aquifer. The reference hydraulic head is equal to zero at top of the aquifer. Similarly, the reference hydraulic head is equal to $\varepsilon * 100$ at the bottom of the aquifer, as $y = 0$. The flow boundary condition is assumed to be constant throughout the ocean face. On the inland face, the reference hydraulic head is varying linearly along the length of the inland face. It can be noted from Figure 2 that the reference hydraulic head is h_d at the left side of inland face of the aquifer, and is decreasing linearly at a rate of $\Delta h/1400$. The boundary condition for the phreatic surface is specified as follows (Galeati *et al.*, 1992):

$$K_{yy}\left(\frac{\partial h}{\partial y} + \varepsilon c\right) = V_\mathrm{r} - S_y \frac{\partial h}{\partial t} \tag{19}$$

where, K_{yy} is the actual hydraulic conductivity in y direction, S_y is the specific yield, V_r is the vertical recharge, c is the salt concentration, h is the reference hydraulic head. The three other faces of the aquifer are impermeable. A zero flux boundary condition is specified for these faces.

The advective mixed outflux can exit through the top 20% portion of the aquifer. In this portion, the concentration gradient normal to the ocean face is equal to zero. In the rest 80% of the ocean face, the solute concentration is equal to one, as it allows influx of saltwater into the aquifer. Freshwater enters the aquifer through the inland face of the aquifer. Therefore, the solute concentration is equal to zero on the inland face. It is considered that zero concentration mass influx occurs through the top phreatic surface, and the advective component of the solute mass influx is equal to zero. Therefore, concentration gradient normal to the phreatic surface becomes zero. The other three faces, front, back, and bottom of the aquifer are impermeable. Hence the solute concentration gradient normal to these aquifer faces is set equal to zero. Steady-state reference hydraulic head and concentration are assumed as the initial condition for transient flow and transport.

Figure 2 shows the locations of the pumping wells. The water is assumed to be pumped only from the vertically middle layer of the aquifer. The pumping rate from the aquifer is considered as transient. A time step of 180 days is considered in case of pumping. The pumping rate is considered constant for each time step of 6 months for a particular well. To train the ANN model, pumping patterns are generated randomly over a period of 3 years, using a uniform distribution. In the illustrative example, the ANN is trained with patterns corresponding to an upper limit of 18 000 m^3/day and a lower limit of 0 m^3/day. The concentration values shown here are the normalized saltwater concentration with a range of (0, 1). The value 1 corresponds to a concentration of 2500 mg/L.

6. Performance Evaluations

The performances of the developed ANN and the simulation – optimization model are evaluated by applying the model to the illustrative study area, as shown in Figure 2. The performances of the developed models are described under two sub-headings, (a) performance evaluation of the ANN model and (b) performance evaluation of the simulation – optimization model.

6.1. PERFORMANCE EVALUATION OF THE ANN MODEL

The primary objective of performance evaluation is to check whether the developed ANN model can be used as an approximator for simulation of three-dimensional density-dependent flow and transport processes in coastal aquifers. The performance of the developed ANN model is evaluated on the basis of relative error and co-efficient of correlation criteria. The relative error (RE) shows the relative differences between actual and predicted salt concentration of the pumped water. The actual salt concentrations are those generated by the numerical simulation model. The predicted salt concentrations are those generated by the developed ANN model. Lesser the value of the relative error, better would be the model performance. Table II lists the relative errors between actual and predicted salt concentrations of the pumped water at different pumping locations. The maximum and minimum relative errors are 6.06 and 0.08%, respectively, with an average of 0.98%. These values are quite low and are in the acceptable range. Figure 3 shows graphical representation of relative errors for different pumping locations.

Coefficient of correlation (R) shows the strength of the relationship between actual and predicted salt concentration of pumped water. High value of the coefficient of correlation (e.g. $R > 95\%$) represents a strong relationship between actual and predicted salt concentrations. Table II lists coefficient of correlation between actual and predicted salt concentrations in the pumped water. The maximum and minimum coefficients of correlation values found are 99.77 and 97.81%, respectively, with an average of 99.41%. These values are encouraging.

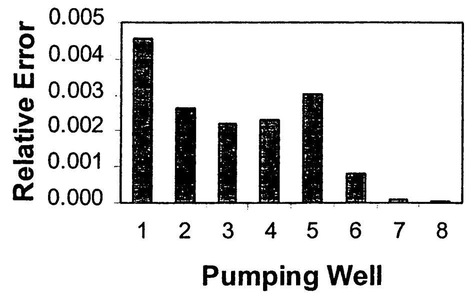
The scatter plots of actual and predicted salt concentrations are shown in Figures 4 and 5 for time steps 2 and 3. The x-axis of Figures 4 and 5 represents actual salt concentration, and the y-axis represents predicted salt concentration.

Table II. Average relative error between the actual and predicted concentrations

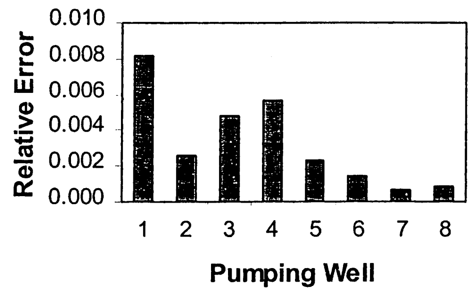
Time step	Pumping well	Relative error (%)	R (%)
1	1	0.49	99.69
	2	0.54	99.57
	3	0.29	99.66
	4	0.51	99.37
	5	0.50	99.35
	6	0.08	99.57
	7	0.08	99.77
	8	0.08	99.56
2	1	1.28	99.46
	2	1.07	99.67
	3	0.86	99.46
	4	1.01	99.47
	5	0.95	99.41
	6	0.25	99.56
	7	0.19	99.69
	8	0.18	99.59
3	1	3.32	98.91
	2	6.06	97.81
	3	1.55	99.08
	4	1.58	99.41
	5	1.58	99.37
	6	0.38	99.47
	7	0.36	99.39
	8	0.29	99.54
Average		0.98	99.41

These plots show the degree of correlation between actual and predicted salt concentrations. It can be observed that the correlation between actual and predicted salt concentration is high, and the scatter plots resemble a straight line with a slope 1:1. Figure 6 shows actual and predicted concentrations in the form of bar chart.

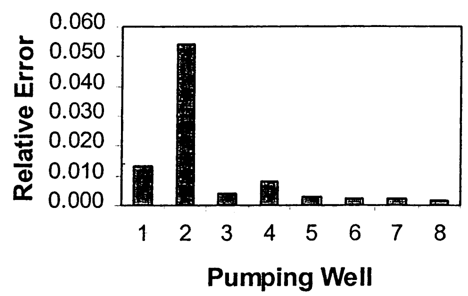
It can be concluded, from these results, that three-dimensional density-dependent flow and transport equations can be approximated by an ANN model with a fair degree of accuracy. The developed ANN model is simple in concept and less computationally intensive, compared to a numerical simulation model. The trained ANN model takes only 2 s CPU time to compute salt concentration of the pumped water on a P-IV (1.7 MHz), 128 MB RAM PC. The trained ANN model can be easily linked with an optimization algorithm to solve a saltwater intrusion management model. The performance of the simulation – optimization approach is also evaluated for this illustrative study area.



(a) For time step 1



(b) For time step 2



(c) For time step 3

Figure 3. Relative error between actual and predicted salt concentrations.

6.2. PERFORMANCE EVALUATION OF THE SIMULATION OPTIMIZATION METHODOLOGY (ANN–GA)

The applicability of the simulation – optimization methodology is evaluated for the illustrative study area. The aquifer is subjected to saltwater intrusion along the coastal face of the aquifer. The hypothetical unconfined aquifer is homogeneous with respect to hydraulic conductivity, molecular diffusion, and longitudinal and transverse dispersitivities. The flow and transport boundary conditions are as discussed earlier, and are shown in Figure 2.

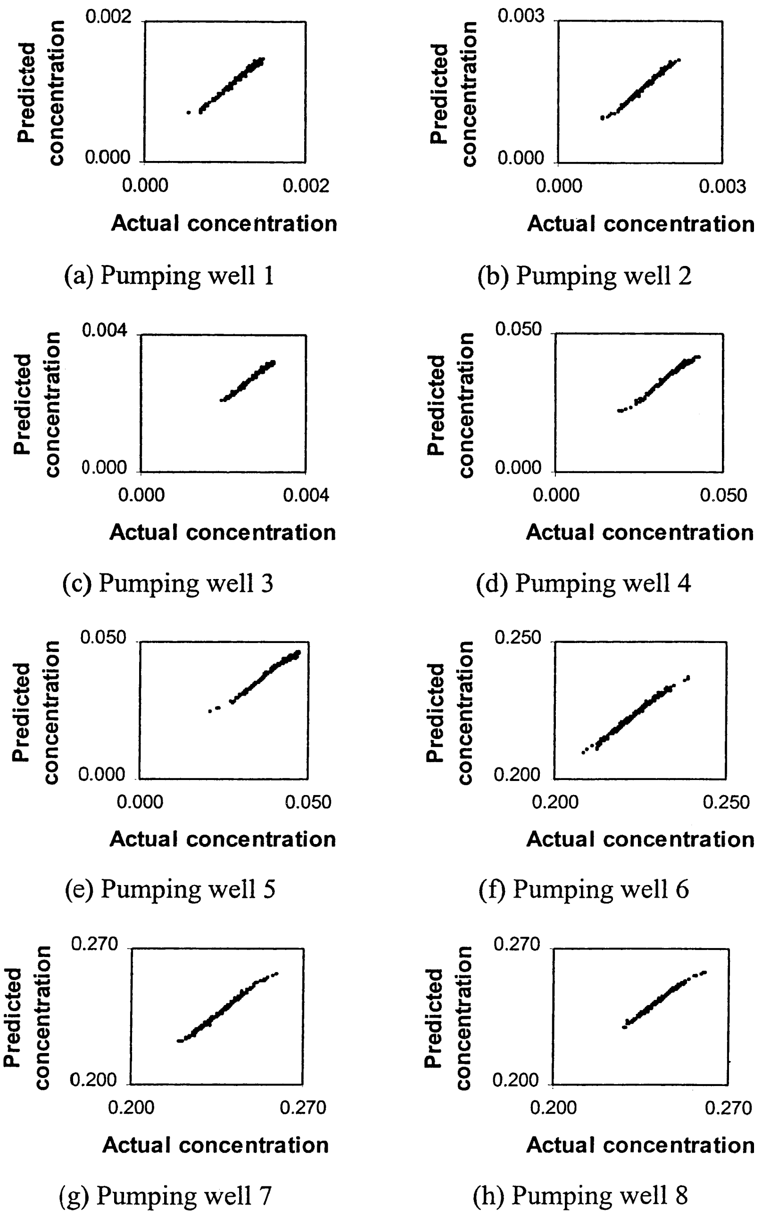
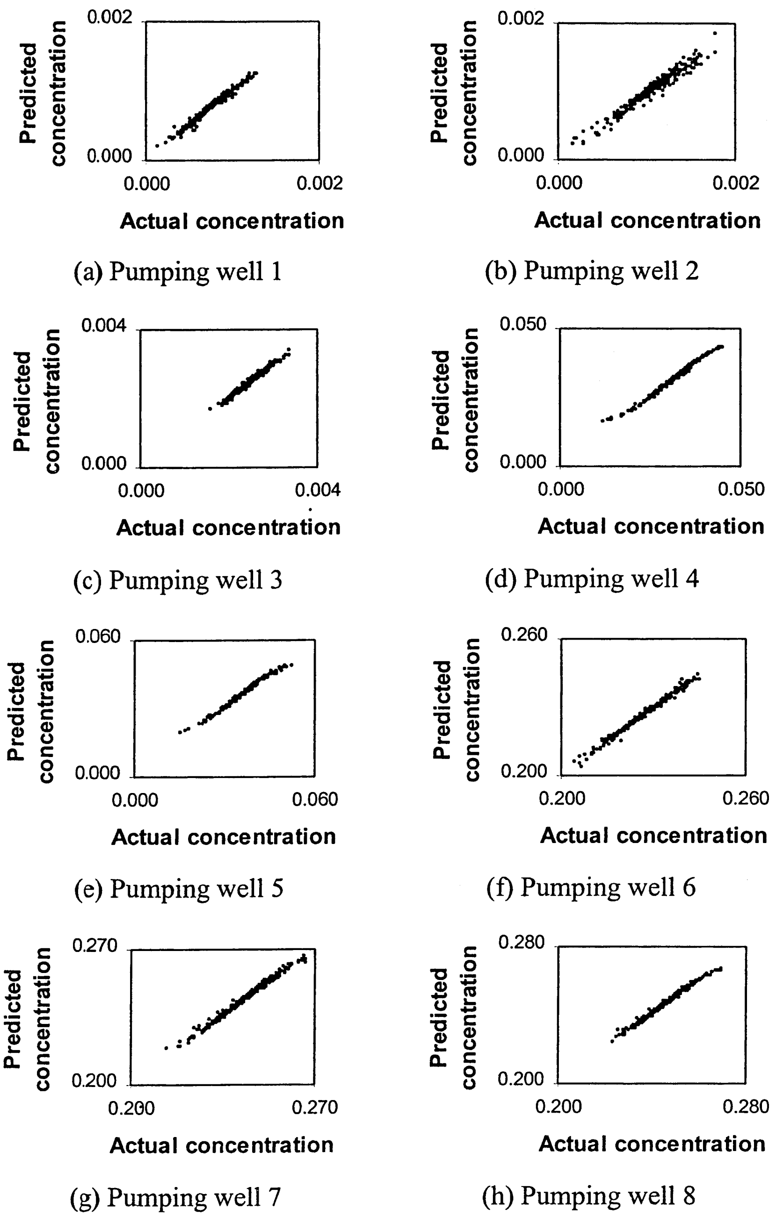


Figure 4. Scatter plot between actual and predicted salt concentration for time step 2.

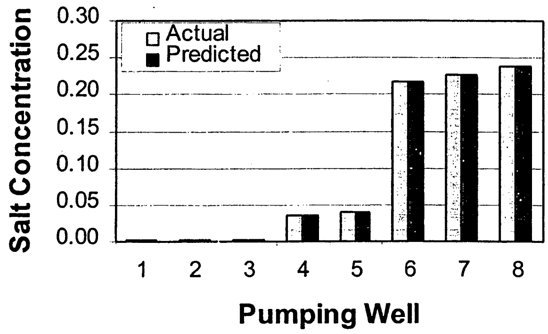
The primary objective of the management model is to maximize freshwater withdrawal for beneficial use from the coastal aquifer, while maintaining salt concentration of the pumped water under specified permissible limits. The fresh water extraction from the aquifer is done from prespecified pumping locations in the aquifer. In this study, eight possible pumping locations are chosen. These pumping



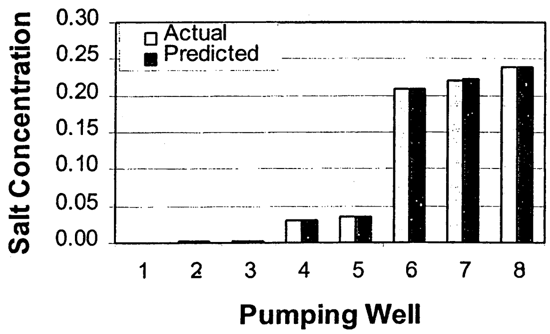
(a) Pumping well 1 (b) Pumping well 2
(c) Pumping well 3 (d) Pumping well 4
(e) Pumping well 5 (f) Pumping well 6
(g) Pumping well 7 (h) Pumping well 8

Figure 5. Scatter plot between actual and predicted salt concentration for time step 3.

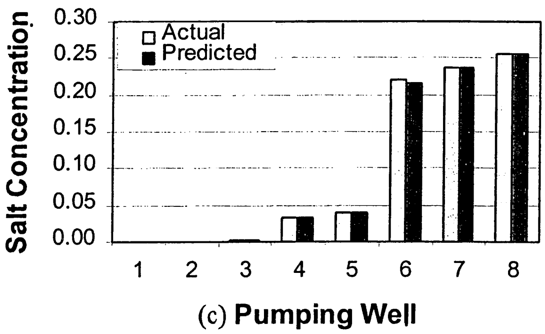
locations are shown in the Figure 2 and are numbered 1 to 8. It is considered that the length of the strainer in each well is 20 m, and these strainers are located at the vertically middle layer of the aquifer. The upper limit of pumping from a possible pumping location is taken as 18 000 m^3/day, and the lower limit is 0 m^3/day. The ANN is also trained with patterns generated using these bounds.



(a) For time step 1



(b) For time step 2



For time step 3

Figure 6. Actual and predicted salt concentrations.

The maximum permissible salt concentration of the pumped water is specified as 0.2373.

The formulated nonlinear saltwater intrusion management model is solved using real coded GA. The real coded GA employs simulated binary crossover (SBX) and parameter-based mutation operators (Deb, 2000) to produce child solutions from parent solutions. The distribution index, n_c for crossover, and η_m for mutation control the creation of child solutions near or far from the parent solutions. A low value of distribution index would create child solutions far away from the parent solutions. On the other hand, a high value would create child solutions near the parent solutions. In this study, the distribution index for crossover is taken as 5, and that for mutation is taken as 30. The probability of crossover (P_c) is taken as 0.85, and the probability of mutation (P_m) is taken as 0.001. The GA code developed at KANGal (Kanpur Genetic Algorithm Laboratory, IIT Kanpur) is used to solve the formulated single objective optimization model.

The trained ANN model is used as the approximate simulator for linking with the GA-based optimization model. The linked simulation – optimization model is solved to obtain the optimal rate of withdrawal for beneficial use from the study area. The optimal withdrawal of water for beneficial use from the costal aquifer is 99 077 m^3/day. These results are obtained after 10 000 iterations of the real coded GA. It is also verified that the obtained solutions do not improve after 10 000 iterations of the real coded GA. It takes about 20 min to complete 10 000 iterations of the real coded GA on a Sun E10000 UltrasparcII workstation. A population size of 800 is used in this study.

The formulated management model is also solved using the embedded optimization technique. In this case, the optimal withdrawal is 99 089 m^3/day. Table III presents optimal solutions found by the ANN–GA model and the solutions obtained using the embedding technique. The optimal amount of total withdrawal obtained as solution from both the models is all most same. However, the optimal pumping rates at different pumping locations obtained as solutions of the ANN–GA model, and as solution of the embedded optimization model are not identical. Considering the objective function and constraints of the saltwater intrusion management problem, the resulting optimization models are non-convex nonlinear in nature (Willis and Finney, 1988). Therefore, it is possible that there are several alternative optimal solutions of the optimization model. It is also possible that the solutions obtained are local optimal solutions. Because, the optimal objective function values representing the total withdrawals from the aquifer are essentially the same, it can be argued that these solutions obtained using two approaches may represent global optimal, but alternate optimal solutions. This if true, would also mean that the optimal pumping rates are not unique. The isochlors and isoheads for the optimal solution using the embedding technique are shown in Figures 7–9 for three different time steps. These isochlors and isoheads are for the middle horizontal layer of the aquifer. It may be observed that the isoheahs do show symmetry. This may be due to the linear variation of hydraulic head along the inland face of the aquifer, combined with the spatial non-uniformity in the pumping rates.

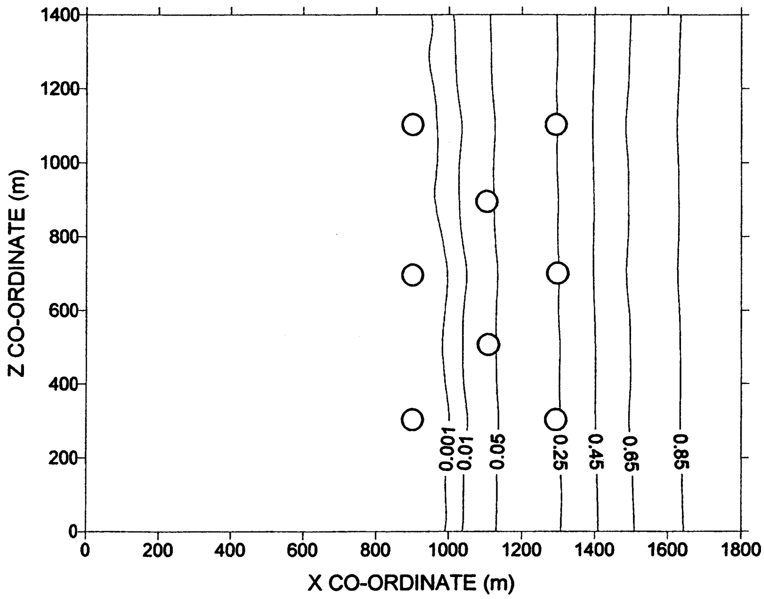
The objective function in the illustrative problem maximizes total pumping from wells 1 to 8. In this particular study area, well numbers 6, 7, and 8 are located near the ocean face. The effect of pumping on saltwater intrusion at ocean face should be lesser, as the distance of pumping wells increases from the ocean face. However, the

Table III. Spatial and temporal distribution of optimal pumping values

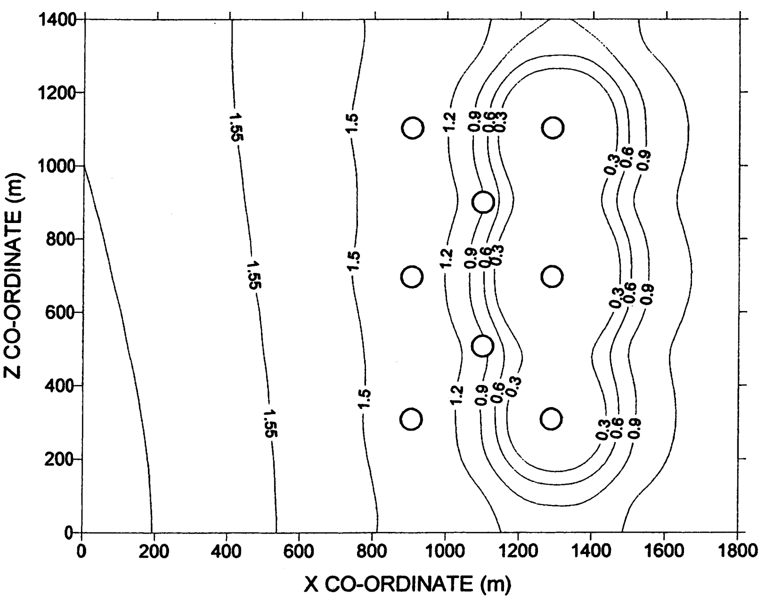
		Optimal pumping rates (m^3/day)	
Time step	Pumping well	ANN–GA model	Embedded technique
1	1	50	0
	2	40	0
	3	3	0
	4	176	0
	5	2	0
	6	8338	10 764
	7	7803	15 192
	8	7273	13 984
2	1	3259	0
	2	231	0
	3	48	0
	4	121	0
	5	8	0
	6	8575	8046
	7	16 845	1499
	8	7174	11 278
3	1	525	2822
	2	221	6372
	3	19	463
	4	36	0
	5	69	0
	6	11 128	12 108
	7	16 520	13 836
	8	10 613	2721
Total		99 077	99 089

optimal solution specifies almost 90 to 95% of the total pumping from these wells, 6 to 8, while satisfying the upper limit on the saline concentration of the pumped water. Because of this, the effect of pumping in the isoheads is more prominent compared to the effect on isochlors. As the hydraulic gradient is more affected in the internal portion of the aquifer due to these patterns of pumping, the affect on isochlors is less prominent. This may results in an optimal solution where isochlors remain rather steady. This phenomenon can be observed in Figures 7–9. It can be also stated that these observations are only valid for the illustrative problem chosen.

The management model using embedded technique has 1915 variables along with 1890 nonlinear constraints, and 24 linear constraints. This model is solved using MINOS (Murtagh and Saunders, 1993). On the other hand, the ANN–GA model has only 24 variables along with 24 constraints. The solution of the management

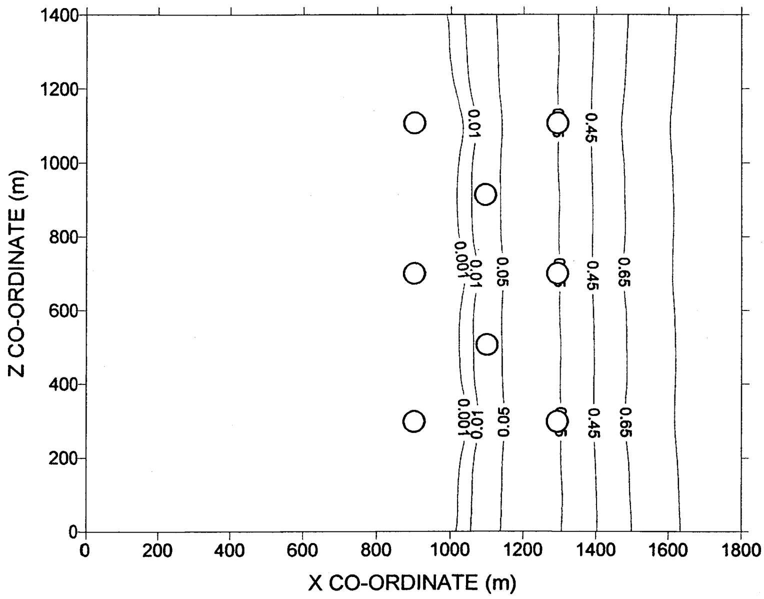


(a) Isochlors

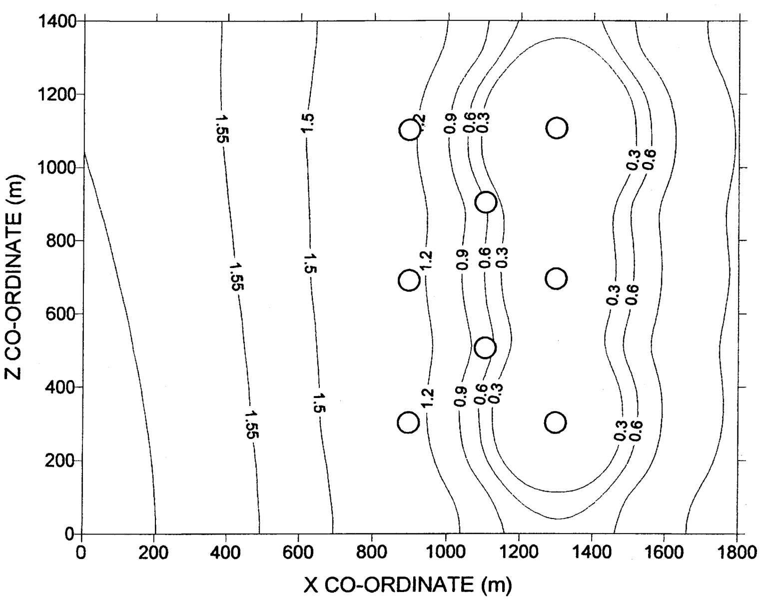


(b) Isoheads

Figure 7. Optimization results: Isochlors and Isoheads at vertically middle layer of the aquifer at time step 1.

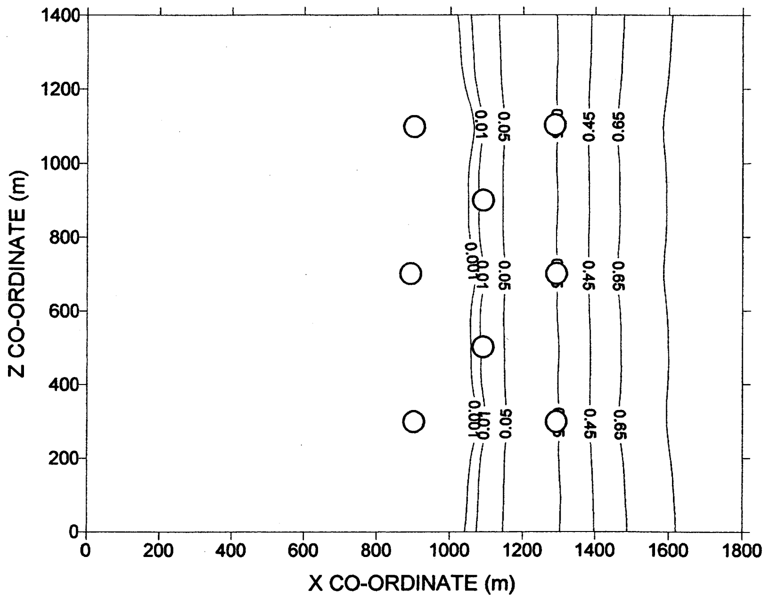


(a) Isochlors

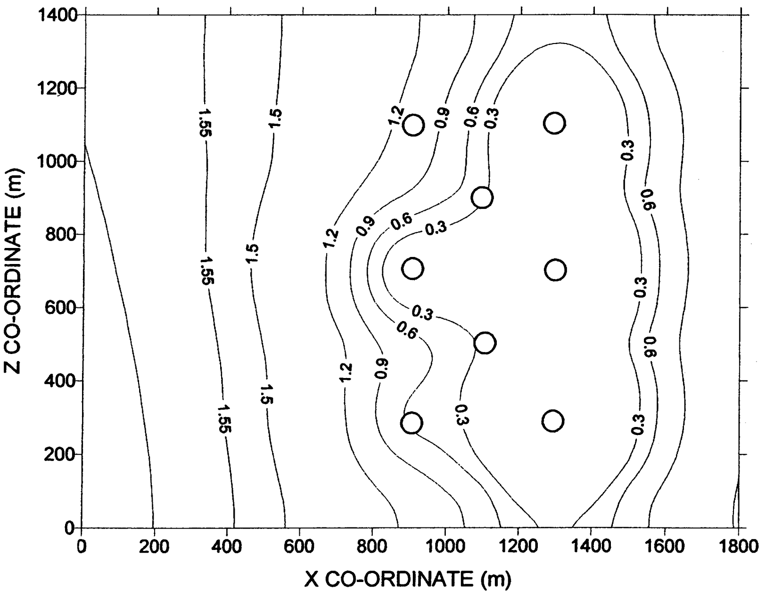


(b) Isoheads

Figure 8. Optimization results: Isochlors and Isoheads at vertically middle layer of the aquifer at time step 2.



(a) Isochlors



(c) Isoheads

Figure 9. Optimization results: Isochlors and Isoheads at vertically middle layer of the aquifer at time step 3.

model using the embedding technique takes 86 hr of CPU time on Sun E10000 UltrasparcII workstation, compared to 20 min of CPU time for the ANN–GA model on the same machine. Therefore, the ANN–GA model requires much less CPU time. However, the amount of information available from the solution results of the embedded model is much more than that from ANN–GA model. For example, the isochlors and the isoheads are obtained from the embedded model solution results only.

7. Conclusion

A linked simulation – optimization methodology is developed for optimal management of saltwater intrusion in coastal aquifers. The three-dimensional transient density-dependent flow and transport processes in coastal aquifer are approximated using a trained ANN model. The trained ANN model is linked with a GA-based optimization model. The ANN model calculates salt concentration of the pumped water at different time steps. The trained ANN model is linked externally with the optimization model. The objective of the management model is to maximize the withdrawal of water for beneficial use from a coastal aquifer, while maintaining salt concentration of the pumped water under specified permissible limits. The formulated optimization model is solved using real coded GA. The performance of the developed methodology is evaluated for an illustrative study area. The results obtained by the proposed simulation – optimization model are compared with the solution results obtained using an embedded optimization model. The optimal total pumping rates obtained from both the models are almost equal, though the individual optimal pumping rates at different pumping locations are not the same. These results may represent alternate optimal solutions. The proposed ANN–GA model is simple in concept and takes considerably less CPU time compared to the embedded-optimization approach. The performance evaluation of the developed ANN–GA model shows its potential applicability to solve saltwater intrusion management problems in coastal aquifers.

No doubt there are some limitations in the developed methodology. The performance of the ANN–GA-based management model would largely depend on the accuracy and adequacy of the ANN model used as an approximate simulator of the flow and transport processes. The number of training patterns required may increase substantially, if heterogeneity of the aquifer parameters is to be incorporated. Also, rigorous performance evaluation would be necessary before the potential applicability of the proposed methodology is fully established.

References

Alley, W. M., 1986, ‘Regression approximation for transport model constraint sets in combined aquifer simulation-optimization studies’, *Water Resour. Res.* **22**(4), 581–586.

Aly, A. H. and Peralta, R. C., 1999a, ‘Optimal design of aquifer cleanup systems under uncertainty using a neural network and genetic algorithms’, *Water Resour. Res.* **35**(8), 2523–2532.

Aly, A. H., and Peralta, R. C., 1999b, 'Comparison of a genetic algorithm and mathematical programming to the groundwater cleanup systems', *Water Resour. Res.* **35**(8), 2415–2425.

Bear, J. and Dagan, G., 1964, 'Some exact solutions of interface problems by means of the hodograph method', *J. Geophys Res.* **69**, 1563–1572.

Cheng, J. M. and Chen, C. X., 2001, 'Three-dimensional modeling of density-dependent saltwater intrusion in multilayered coastal aquifers in Jahe river basin, Shandong province, China', *Ground Water*, **39**(1), 137–143.

Cieniawski, S. E., Eheart, J. W. and Ranjithan, S., 1995, 'Using genetic algorithms to solve a multi-objective groundwater monitoring problem', *Water Resour. Res.* **31**(2), 399–409.

Das, A. and Datta, B., 1999a, 'Development of management models for sustainable use of coastal aquifers', *J. Irrg. Drainage Eng. ASCE* **125**(3), 112–121.

Das, A. and Datta, B., 1999b, 'Development of multiobjective management models for coastal aquifers', *J. Water Resour. Plan. Manage. ASCE.* **125**(2), 76–87.

Das, A. and Datta, B., 2000, 'Optimization based solution of density-dependent seawater intrusion in coastal aquifers', *J. Hydrol. Eng.* **5**(1), 82–89.

Deb, K., 2000, 'An efficient constraint handling method for genetic algorithms', *Comput. Methods Appl. Mech. Eng.* **186**, 311–338.

Deb, K., 2001, *Multi-Objective Optimization Using Evolutionary Algorithms*, Wiley, UK.

Ejaz, M. S. and Peralta, R. C., 1985, 'Modeling for optimal management of agricultural and domestic wastewater loading to streams', *Water Resour. Res.* **31**(4), 1087–1096.

Emch, P. G. and Yeh, W. W.-G., 1998, 'Management model for conjunctive use of coastal surface water and ground water', *J. Water Resour. Plan. Manage. ASCE* **124**(3), 129–139.

Essink, G. H. P. O., 2001, 'Saltwater intrusion in 3D Large Scale aquifers: A Dutch case' *Phys. Chem. Earth* **26**(4), 337–344.

Galeati, G., Gambolati, G. and Neuman, S. P., 1992, 'Coupled and partially coupled Eulerian–Lagrangian model for freshwater–seawater mixing', *Water Resour. Res.* **28**(1), 147–165.

Galeati, G., Gambolati, G. and Neuman, S. P. 1992, 'Coupled and partially coupled Eulerian–Lagrangian model for freshwater–seawater mixing', *Water Resour. Res.* **28**(1), 147–165.

Goldberg, D. E., 2000, *Genetic Algorithms in Search, Optimization, and in Machine Learning*, *Addison Wiley*, Bangalore, India.

Gorelick, S. M., 1983, 'A review of distributed parameter groundwater management modeling methods', *Water Resour. Res.* **19**(2), 305–319.

Hantush, M. S., 1968, 'Unsteady movement of freshwater in thick unconfined saline aquifers', *Bull. Int. Assoc. Sci. Hydrol.* **XIII**(2), 40–60.

Henry, H. R., 1959, 'Salwater intrusion into freshwater aquifers', *J. Geophys. Res.* **64**, 1911–1919.

Holland, J. H., 1975, *Adaptation in Natural and Artificial Systems*, University of Michigan Press, Michigan.

Huyakorn, P. S., Andersen, P. F., Mercer, J. W. and White H. O., 1987, 'Saltwater intrusion in aquifers: Development and testing of a three-dimensional finite element model', *Water Resour. Res.* **23**(2), 293–312.

Johnson, V. M. and Rogers, L. L., 2000, 'Accuracy of neural network approximations in simulation–optimization', *J. Water Resour. Plan. Manage. ASCE* **126**(2), 48–56.

Liu, P. L.-F., Cheng, J. A. and Lee, J. H., 1981, 'Boundary integral equation solutions of moving interface between two fluids in porous media', *Water Resour. Res.* **17**(5), 1445–1452.

Lefkoff, L. J. and Gorelick, S. M., 1990, 'Simulating physical processes and economic behavior in saline, irrigated agriculture: Model develpment', *Water Resour. Res.* **26**(7), 1359–1369.

McKinney, D. C., and Lin, M.-D., 1994, 'Genetic algorithms solution of groundwater management models', *Water Resour. Res.* **30**(4), 1897–1906.

Mercer, J. W., Larson, S. P. and Faust, C. R., 1980, 'Simulation of saltwater interface motion', *Ground Water* **18**(4), 374–385.

Morshed, J. and Kaluarachchi, J. J., 1998, 'Application of artificial neural networks and genetic algorithms in flow and transport simulation', *Adv. Water Resour*. **22**(2), 145–158.

Morshed, J. and Kaluarachchi, J., 2000, 'Enhancements to genetic algorithm for optimal ground-water management', *J. Hydrol. Eng. ASCE* **5**(1), 67–73.

Murtagh, B. A. and Saunders, M. A., 1993, 'MINOS 5:4 user's guide, technical report, SOL 83-20R', *Systems Optimization Laboratory, Department of Operation Research, Stanford University*, Stanford, California, 94305–4022.

Pinder, G. F. and Page, R. H., 1977, 'Finite element simulation of salt water intrusion on the South Fork of Long Island', *Proceedings of the 1st International Conference on Finite Elements in Water Resources*, Pentech Press, London, pp. 2.51–2.69.

Putti, M. and Paniconi, C., 1995, 'Picard and Newton linearization for the coupled model of saltwater intrusion in aquifers', *Adv. Water Resour.* **18**(3), 159–170.

Ritzel, B. J., Eheart, J. W. and Ranjithan, S., 1994, 'Using genetic algorithms to solve a multiple objective groundwater pollution containment problem', *Water Resour. Res.* **30**(5), 1589–1603.

Rogers, L. L. and Dowla, F. U., 1994, 'Optimization of ground water remediation using artificial neural networks and parallel solute transport modeling', *Water Resour. Res.* **30**(2), 457–481.

Rosenwald, G. W., and Green, D. W., 1974, 'A method for determining the optimal location of wells in a reservoir using mixed-integer programming', *Soc. Res. Eng. J.* **14**, 44–54.

Shamir, U. and Dagan, G., 1971, 'Motion of the seawater interface in coastal aquifers: A numerical solution', *Water Resour. Res.* **7**(3), 644–657.

Simpson, M. J. and Clement, T. P., 2003, 'Theoretical analysis of the worthiness of Henry and Elder problems as bench Marks of density-dependent groundwater flow model', *Adv. Water Resour.* **26**(1), 17–31.

Strack, O. D. L., 1976, 'A single-potential solution for regional interface problems in coastal aquifers', *Water Resour. Res.* **12**(6), 1165–1174.

Taigbenu, A. E., Liggett, J. A. and Cheng, A. H. D., 1984, 'Bioundary integral solution to seawater intrusion into coastal aquifers', *Water Resour. Res.* **20**(8), 1150–1158.

Willis, R. and Finney, B. A., 1988, 'Planning model for optimal control of saltwater intrusion', *J. Water Resour. Plan. Manage. ASCE* **114**(2), 163–178.