Optimal Management of Freshwater Lens in a Small Island Using Surrogate Models and Evolutionary Algorithms

Behzad Ataie-Ashtiani¹; Hamed Ketabchi²; and Mohammad Mahdi Rajabi³

Abstract: This paper examines a linked simulation-optimization procedure based on the combined application of an artificial neural network (ANN) and genetic algorithm (GA) with the aim of developing an efficient model for the multiobjective management of groundwater lenses in small islands. The simulation-optimization methodology is applied to a real aquifer in Kish Island of the Persian Gulf to determine the optimal groundwater-extraction while protecting the freshwater lens from seawater intrusion. The initial simulations are based on the application of SUTRA, a variable-density groundwater numerical model. The numerical model parameters are calibrated through automated parameter estimation. To make the optimization process computationally feasible, the numerical model is subsequently replaced by a trained ANN model as an approximate simulator. Even with a moderate number of input data sets based on the numerical simulations, the ANN metamodel can be efficiently trained. The ANN model is subsequently linked with GA to identify the nondominated or Pareto-optimal solutions. To provide flexibility in the implementation of the management plan, the model is built upon optimizing extraction from a number of zones instead of point-well locations. Two issues are of particular interest to the research reported in this paper are: (1) how the general idea of minimizing seawater intrusion can be effectively represented by objective functions within the framework of the simulation-optimization paradigm, and (2) the implications of applying the methodology to a real-world small-island groundwater lens. Four different models have been compared within the framework of multiobjective optimization, including (1) minimization of maximum salinity at observation wells, (2) minimization of the root mean square (RMS) change in concentrations over the planning period, (3) minimization of the arithmetic mean, and (4) minimization of the trimmed arithmetic mean of concentration in the observation wells. The latter model can provide a more effective framework to incorporate the general objective of minimizing seawater intrusion. This paper shows that integration of the latest innovative tools can provide the ability to solve complex real-world optimization problems in an effective way. DOI: 10.1061/(ASCE)HE.1943-5584.0000809, © 2014 American Society of Civil Engineers.

Author keywords: Seawater intrusion; Freshwater lens; Numerical modeling; Artificial neural networks; Genetic algorithm; Multiobjective analysis; Persian Gulf.

Introduction

Groundwater scarcity looms as an increasingly critical issue in coastal aquifers around the world. This is mostly due to the fact that more than half of the world’s population is living within 60 km of the shoreline and this could rise to three-quarters of the world’s population by the year 2020 (United Nations Conference on Environment, and Development 1992). A lowered water table as a result of overexploitation may induce seawater to reverse flow toward the land and hence initiate seawater intrusion. This results in the most prominent type of groundwater pollution in coastal aquifers (Ataie-Ashtiani et al. 1999; Wheater et al. 2010). Well-known examples are coastal aquifers in India, China, the Gaza strip, California, and Spain. Many small islands around the world contain a unique form of coastal aquifer system described as fresh-groundwater lenses, relatively thin veneers of fresh groundwater overlying seawater in highly permeable aquifers (White et al. 1999; Van der Velde et al. 2007; Ataie-Ashtiani et al. 2013a). These freshwater lenses are some of the most vulnerable coastal aquifer systems in the world (White and Falkland 2010). These resources of small islands can be highly at risk of climate change impacts, including sea-level rise and recharge variations (Ketabchi et al. 2013).

Under natural conditions, salinity caused by seawater intrusion will remain in a coastal aquifer system for an accordingly long period. Remediation is expensive and often inefficient (Park and Aral 2008; Wheater et al. 2010; Park et al. 2012). Therefore, it is critically important to prevent seawater intrusion by managing withdrawals to prevent overuse of sustainable yields. A novel approach in designing sustainable groundwater-extraction schemes in coastal aquifer systems is to combine a seawater-intrusion simulator with an optimization algorithm. The physics of seawater intrusion are rather well-understood and a variety of modeling approaches exist (Milnes and Renard 2004; Werner et al. 2013). In the linked simulation-optimization process, seawater intrusion can be simulated through analytical models (e.g., Cheng et al. 2000; Mantoglou 2003; Park and Aral 2004; Ataie-Ashtiani et al. 2013b), sharp-interface numerical models (e.g., Finney et al. 1992; Emch and Yeh 1998; Rao et al. 2003; Ataie-Ashtiani and Ketabchi 2011), density-dependent numerical models (e.g., Ataie-Ashtiani et al. 1999; Das and Datta 2000; Qahman et al. 2005; Kourakos and Mantoglou 2009), and surrogate or metamodels.
In general, choice of the appropriate optimization algorithm is highly influenced by the nonlinear, nonconvex, and sometimes even nondifferentiable or discontinuous nature of coastal aquifer-management problems. Linear programming (e.g., Shamir et al. 1984), nonlinear programming (e.g., Emch and Yeh 1998), and a number of evolutionary algorithms [such as the evolutionary annealing simplex scheme (e.g., Kourakos and Mantoglou 2009), genetic algorithm (GA) (e.g., Mantoglou et al. 2004; Dhar and Datta 2009a) and ant colony optimization (e.g., Ataie-Ashtiani and Ketabchi 2011)] have been used in optimizing groundwater-extraction. A survey of the literature published in the past few years shows a growing trend towards the use of evolutionary algorithms in coastal aquifer-management problems. The GA is arguably the most popular of evolutionary algorithms (Nicklow et al. 2010; Werner et al. 2013).

Even though the underlying objective of the optimization model in most coastal aquifer-management problems presented in the literature are the same (i.e., increase fresh-groundwater extraction while reducing seawater intrusion), the mathematical representation can vary. The former objective can be achieved by maximizing a function that represents the total pumping rate, or it can be embodied in constraints on maximum and minimum pumping rates. The latter objective can be characterized by minimizing functions that represent the volume of seawater that penetrates the aquifer, the draw-down, the distance of the stagnation point, the pumped-water salinity, or the deviation from the target concentration. Constraints on toe location, interface elevation at a particular location, groundwater heads, flow potential, and salt concentration of the pumped water can also be used to fulfill the latter objective (e.g., Cheng et al. 2000; Mantoglou 2003; Park and Aral 2004; Qahman et al. 2005; Dhar and Datta 2009a, b; Bhattacharjya and Datta 2005, 2009; Sreekanth and Datta 2010, 2011; Ataie-Ashtiani and Ketabchi 2011).

The linked simulation-optimization procedure provides several key advantages. First, it can account for the complex and nonlinear behavior of the groundwater system. Second, if the method is properly applied, a universal optimum solution can be provided. This is in contrast with methods based on shear comparison of simulation results for various extraction scenarios, which only identify the best option among the set of simulated alternatives. Third, this methodology can result in policymaking prior to the initiation of seawater intrusion. However, the performance of this approach is highly dependent on the precision of the simulator, efficacy of the optimization engine, computational efficiency of linked simulation-optimization process, applicability of the management strategy, and how well the overall strategy is being represented by the objective function(s) and the constraints (Bhattacharjya and Datta 2005; Dhar and Datta 2009a; Ataie-Ashtiani and Ketabchi 2011).

Previous research has obtained optimal solutions of coastal aquifer-management problems at varying degrees of success (Ataie-Ashtiani and Ketabchi 2011). Most of the previous studies have focused on hypothetical aquifers or small-scale field problems with substantial simplifying assumptions that in some cases undermine the integrity of the management model. For example, assuming a sharp interface between freshwater and seawater may produce erroneous results in some real-world problems in which a large transition-zone exists between the two phases. In contrast, employing the more sophisticated density-dependent models may render the linked simulation-optimization process computationally infeasible. To solve this problem, the research reported in this paper examines a procedure in which a density-dependent numerical model is substituted by a trained artificial neural network (ANN) model with comparable results. The objective is to provide an efficient simulation-optimization model for multiobjective management of small-island aquifer systems. The emphasis is on the applicability of the employed methodology in real-world problems in terms of both computational efficiency and flexibility in performance. The next sections provide a concise description on the theoretical background of the simulation-optimization model and describe an application of the methodology for a small-island aquifer system. Kish Island, in the Persian Gulf, is the case study of the research reported in this paper.

Methodology

A novel methodology is developed to integrate simulation model in the framework of a management paradigm for obtaining practical extraction strategies. In many similar studies, the optimization model eventually results in the establishment of the following results: (1) location of the pumping wells (e.g., Park and Aral 2004) either chosen from a fixed pool of predetermined well locations or determined based on model spatial discretization, and (2) the extraction rate for each of the pumping wells (e.g., Bhattacharjya and Datta 2005, 2009; Dhar and Datta 2009a; Ataie-Ashtiani and Ketabchi 2011). In a region where land is primarily owned by numerous individuals, it is mainly the water-consumers that determine the well locations based on practical limitations (e.g., presence of obtrusive structures) and economic interests (e.g., minimizing piping and drilling costs). A management plan that imposes certain pumping-well locations and ascribes fixed pumping-rates to these wells, without considering the interests of water-consumers, is somewhat impractical. Nonetheless, quantifying water-consumer interests and subsequently reflecting them in the management model is a difficult task. A way to go around this problem is to define extraction zones instead of well-pumping. This provides a high degree of flexibility in implementing the management plan. As soon as the extraction rate for each zone has been determined through the linked simulation-optimization procedure, the local water authorities and consumers can then decide how to ascribe each zone’s share of groundwater extraction to various consumers and the distribution can change over time. In this paper, the management model is built upon optimizing extraction from a number of zones instead of point-well locations.

Available literature such as Bhattacharjya and Datta (2009), Dhar and Datta (2009a), and Sreekanth and Datta (2010, 2011) suggests that there are scopes for development of methodologies, which can generate the nondominated front for multiobjective management of seawater intrusion in coastal aquifers by incorporating density-dependent flow and transport processes. There are also scopes for improving the computational feasibility of linked simulation-optimization by using metamodels for approximation of the physical processes.

The simulation-optimization model developed in this paper for the optimum coastal-aquifer management includes three primary components, as follow: (1) numerical model that simulates the density-dependent flow and solute transport processes associated with seawater intrusion, (2) trained ANN to approximate salinity in the selected observation wells based on different net recharge rates, and (3) optimal search technique based on GA. Fig. 1 represents a schematic flowchart of the linked simulation-optimization model. The seawater intrusion process is initially simulated by employing the SUTRA (Voss and Provost 2010) numerical code (Fig. 1). Directly embedding the numerical simulator in the optimization algorithm is computationally infeasible unless massive
parallel computing facilities are employed. To render the optimization process computationally efficient, the numerical model is subsequently replaced by a trained ANN model as an approximate simulator. The ANN model is then linked with the GA in the framework of four multiobjective optimization paradigms. The entire simulation-optimization (ANN-GA) process for each of the four management models takes only a few minutes to complete. Optimization is terminated after 100 generations are reached (user defined). The theoretical basis of each of the three main components of the simulation-optimization model is briefly described in the next sections.

**Numerical Model**

The SUTRA model is used for numerical simulations. The SUTRA model is a numerical solver of two general balance equations for variable-density single-phase saturated-unsaturated flow and single-species solute transport. The model employs a three-dimensional (3D) Galerkin finite-element approximation of the governing equations in space and an implicit finite-difference approximation in time (Voss and Provost 2010). Automatic calibration is employed to calibrate the numerical model. The procedure is carried out by the automated parameter estimation (PEST) code (Doherty 2005). The PEST code performs inverse modeling by calculating parameter values that minimize a weighted least-squares objective function in the parameter space is calculated. Derivatives of observations with respect to parameters are calculated using finite differences (Doherty 2005). Fig. 2 illustrates the automatic calibration process based on Ataie-Ashtiani et al. (2013a). The parameters that are employed in the SUTRA formulation are \( \rho = \) fluid density; \( S_{\mu p} = \) specific pressure; \( p = \) fluid pressure; \( t = \) time; \( \varepsilon = \) aquifer volumetric porosity; \( c = \) solute concentration (mass solute/mass fluid); \( k = \) solid matrix permeability; \( \mu = \) fluid dynamic viscosity; \( g = \) gravitational acceleration; \( Q_p = \) fluid mass sink or source; \( v = \) average fluid velocity; \( D_m = \) apparent molecular diffusion coefficient; \( I = \) identity tensor; \( D = \) mechanical dispersion tensor; and \( c^* = \) concentration of solute in the source fluid (Voss and Provost 2010). The parameters utilized in formulas related to the PEST inverse code are \( r_i = \) (the \( i \)th residual), which expresses the difference between the model outcome and actual field measurement for the \( i \)th observation; \( w_i = \) observation weight; \( m = \) number of observations; and \( \phi = \) optimal parameter set for which the sum of the squared deviations between the model-generated observations and field observations is reduced to a minimum. Furthermore, \( \mathbf{b}_i \) is a vector of the \( i \)th simulation results; \( x_j \) is the \( j \)th parameter; \( J_{ij} \) is the derivative of the \( i \)th observation with respect to the \( j \)th parameter; \( \alpha = \) Marquardt parameter; \( \mathbf{I} = n \times n \) identity matrix; \( \mathbf{r} = \) vector of residuals for the current parameter set; and \( \mathbf{J} \) is the Jacobian matrix (Doherty 2005). For further detail on SUTRA, the reader is referred to Voss and Provost (2010). More information on the mathematical background of the PEST inverse code is provided in Doherty (2005). Details on the conceptual and numerical model
PROOF

Artificial Neural Network Model

Approximation surrogates have previously been used to replace numerical simulation models. Widely used surrogate models are ANN and more recently genetic programming (GP) (Sreekanth and Datta 2010, 2011). This paper evaluates ANN as a potential surrogate modeling tool for real-world 3D density-dependent models of seawater intrusion. Artificial neural networks learn from data examples presented to them with the aim of capturing the functional relations among the data even if the underlying relationships are unknown or the physical meaning is difficult to explain (Shahin et al. 2008). Once the ANN is trained, the relationship between the inputs and outputs is encoded in the network. It can then be used to predict the output based on the information fed to the input nodes (Bhattacharjya et al. 2007).

A number of studies using ANN models for seawater intrusion simulations showed that if enough information can be provided for ANN training (regarding both the number of samples and the range of the data) the accuracy of ANN results would be comparable with the original numerical model used for training. For instance, Bhattacharjya et al. (2007) presented an ANN model-development methodology to simulate complex transient 3D flow and transport processes in coastal aquifers. The training and testing patterns were generated using a finite-element based numerical model (FEMWATER) and the performance of the developed ANN model was evaluated for a study area consisting of a hypothetical confined aquifer. Bhattacharjya and Datta (2005) developed a linked simulation-optimization model for optimal management of seawater intrusion in coastal aquifers by employing an ANN metamodel to estimate salt concentration of the pumped waters at different time-steps. The performance of the developed optimization model was evaluated using an illustrative hypothetical study area. The evaluation results showed the potential applicability of the developed methodology using a GA-ANN-based linked optimization-simulation model. Similar methodologies were implemented in Bhattacharjya and Datta (2009) and Dhar and Datta (2009a). Kourakos and Mantoglou (2009) presented an optimization method based on modular neural networks (MNN), in which several subnetwork modules, trained using a fast adaptive procedure, collaborate to solve a complex pumping-optimization problem with many decision variables. The numerical code SEAWAT was employed for solving the partial differential equations of flow and density-dependent transport. The modular subnetwork implementation resulted in significant reduction in CPU time and resulted in a better solution than the original numerical model. Banerjee et al. (2011) evaluated the prospect of ANN simulation over mathematical modeling in Kavaratti Island aquifer, located on the west
Table 1. Artificial Neural Network Models Information Utilized in Seawater Intrusion Simulation as a Metamodel in the Literature

<table>
<thead>
<tr>
<th>T1:1</th>
<th>Reference</th>
<th>Type of ANN architecture</th>
<th>ANN architecture design method</th>
<th>Transfer function</th>
<th>Number of patterns</th>
<th>Set of data for input layer</th>
<th>Set of data for output layer</th>
<th>Simulation model, used for pattern-generation</th>
<th>Application</th>
</tr>
</thead>
<tbody>
<tr>
<td>T1:2</td>
<td>Rao et al. (2003)</td>
<td>Back-propagation feed-forward</td>
<td>Three-layer</td>
<td>Trial-and-error evaluation</td>
<td>Sigmoidal</td>
<td>5,000</td>
<td>Pumping values in wells</td>
<td>SHARP numerical model</td>
<td>Hypothetical area, 50 km²</td>
</tr>
<tr>
<td>T1:3</td>
<td>Rao et al. (2004)</td>
<td>Back-propagation feed-forward</td>
<td>24-6-6</td>
<td>Trial-and-error evaluation</td>
<td>Sigmoidal</td>
<td>4,900</td>
<td>Pumping and recharge values in wells</td>
<td>SEAWAT numerical model</td>
<td>Hypothetical area, 2.64 km²</td>
</tr>
<tr>
<td>T1:4</td>
<td>Bhattacharjya and Datta (2005)</td>
<td>Standard back-propagation feed-forward</td>
<td>24-6-24&lt;sup&gt;a&lt;/sup&gt;</td>
<td>Trial-and-error evaluation</td>
<td>Unipolar sigmoidal</td>
<td>2,400</td>
<td>Pumping values in wells</td>
<td>Concentration values in wells</td>
<td>Numerical model</td>
</tr>
<tr>
<td>T1:5</td>
<td>Bhattacharjya et al. (2007)</td>
<td>Standard back-propagation feed-forward</td>
<td>18-6-18&lt;sup&gt;b&lt;/sup&gt;</td>
<td>Trial-and-error evaluation based on RMS error and R</td>
<td>Unipolar sigmoidal</td>
<td>636</td>
<td>Pumping and recharge values in wells</td>
<td>Concentration values in wells</td>
<td>FEMWATER numerical model</td>
</tr>
<tr>
<td>T1:6</td>
<td>Dhar and Datta (2009a)</td>
<td>Standard back-propagation feed-forward</td>
<td>33-66-24</td>
<td>Trial-and-error evaluation</td>
<td>Hyperbolic</td>
<td>3,600</td>
<td>Pumping values in wells</td>
<td>Concentration values in wells</td>
<td>FEMWATER numerical model</td>
</tr>
<tr>
<td>T1:7</td>
<td>Kourakos and Mantoglou (2009)</td>
<td>Feed-forward</td>
<td>34-34-34</td>
<td>Trial-and-error evaluation</td>
<td>—</td>
<td>273</td>
<td>Pumping values in wells</td>
<td>Concentration values in wells</td>
<td>SEAWAT numerical model</td>
</tr>
<tr>
<td>T1:8</td>
<td>Bhattacharjya and Datta (2009)</td>
<td>Standard back-propagation feed-forward</td>
<td>33-28-24</td>
<td>Trial-and-error evaluation based on RMS error and R</td>
<td>Unipolar sigmoidal</td>
<td>2,400</td>
<td>Pumping and recharge values in wells</td>
<td>Concentration values in wells</td>
<td>Numerical model</td>
</tr>
<tr>
<td>T1:9</td>
<td>Seekanth and Datta (2010)</td>
<td>Standard back-propagation feed-forward</td>
<td>33-33-1</td>
<td>Trial-and-error evaluation</td>
<td>Sigmoidal</td>
<td>180</td>
<td>Pumping values in wells</td>
<td>Concentration values in wells</td>
<td>FEMWATER numerical model</td>
</tr>
<tr>
<td>T1:10</td>
<td>Seekanth and Datta (2011)</td>
<td>Back-propagation</td>
<td>33-3-3&lt;sup&gt;c&lt;/sup&gt;</td>
<td>Trial-and-error evaluation</td>
<td>Sigmoidal</td>
<td>230</td>
<td>Pumping values in wells</td>
<td>Concentration values in wells</td>
<td>FEMWATER numerical model</td>
</tr>
<tr>
<td>T1:11</td>
<td>Banerjee et al. (2011)</td>
<td>Feed-forward</td>
<td>1-1-1&lt;sup&gt;d&lt;/sup&gt;</td>
<td>Trial-and-error evaluation</td>
<td>—</td>
<td>—</td>
<td>Pumping values in wells</td>
<td>Concentration values in wells</td>
<td>Field data compared with SUTRA</td>
</tr>
<tr>
<td>T1:12</td>
<td>Present work</td>
<td>Feed-forward</td>
<td>11-40-20</td>
<td>Trial-and-error evaluation</td>
<td>Log-sigmoid</td>
<td>56</td>
<td>Net recharge rate to managerial zones</td>
<td>Concentration values in wells</td>
<td>SUTRA numerical model</td>
</tr>
</tbody>
</table>

Note: R = coefficient of correlation.

<sup>a</sup>Number of neurons in the hidden layer, dependent on the complexity and nonlinearity of the problem, obtained by trial-and-error.

<sup>b</sup>Number of neurons in the hidden layer (approximately 15–25), dependent on the complexity and nonlinearity of the problem, obtained by trial-and-error.

<sup>c</sup>Number of neurons in the hidden layer, determined by trial-and-error.

<sup>d</sup>Number of neurons in the hidden layer (approximately 2–4), dependent on the complexity of the modeling problem and objective of the researcher.
coast of India. The results suggested that ANN models can be simpler and yet accurate alternative to the numerical model. Table 1 summarizes notable ANN model applications as meta-models in seawater intrusion simulations presented to date in the literature.

Fig. 3 shows a three-layer, feed-forward ANN for simulating an input-output response. In the input layer, one neuron is assigned to each input component. No signal is processed in the input layer; however, in the two remaining layers the signal value is updated through the mathematical expression

\[ y_j = \sum_{i=1}^{N} w_{ij}x_i + b_j \]

where \( x_i \) is \( i \)th nodal value in the previous layer; \( y_j \) is \( j \)th nodal value in the present layer; \( b_j \) is bias of the \( j \)th node in the present layer; \( w_{ij} \) is a weight connecting \( x_i \) and \( y_j \); \( N \) is number of nodes in the previous layer; and \( f \) is the activation or transfer function in the present layer (Yoon et al. 2011). The bias is used to scale the input to a useful range to improve the convergence properties of the neural network (Shahin et al. 2008).

Most previous studies focused on hypothetical illustrative areas (Table 1). Generally, the main approach used for the architectural design of ANN models is trial-and-error evaluation. A survey of literature also implies that the following: (1) feed-forward networks are the most commonly used type of ANN for simulation purposes in water-resources engineering applications including forecasting of seawater intrusion, (2) in most cases of practical interest fully connected networks are used, (3) optimal network geometry is highly problem-dependent, (4) smaller networks are generally more favored (this applies to both the number of layers and number of hidden nodes), and (5) one hidden layer is adequate in the approximation of any continuous function. However, the use of more than one hidden layer results in further flexibility at the cost of significantly lengthening the training process (Gümrah et al. 2000; Maier and Dandy 2000; Lallahem et al. 2005; Manisha et al. 2008; Shahin et al. 2008; Kourakos and Mantoglou 2009). As described subsequently in the paper, these general conclusions are used to design the ANN architecture.

Genetic Algorithm Model

Genetic algorithms are a class of heuristic search methods based on natural selection. The concepts of GA are simple. A GA involves three basic mechanisms (initialization, selection, and reproduction) and a set of termination criteria. The termination criteria are especially needed since GA is a stochastic search method that could in principle run forever (Reeves and Rowe 2003). Genetic algorithms can be considered as parallel equivalents of the more conventional serial optimization techniques. The logic behind this notion is that GAs move from entire populations of possible solution to new populations instead of the more classic approach of testing one point after another in the solution phase-space. In multiobjective optimization, the aim is not to find an absolute optimal solution but to seek the set of solutions that are better than all other solutions in at least one objective (Fig. 4). These values are termed nondominated or Pareto-optimal solutions (Kollat and Reed 2006; Kentel and Aral 2007).

Application

The simulation and optimization methodology is applied to a real case study of an unconfined coastal aquifer in Kish Island in the Persian Gulf to determine the optimal extraction rates while protecting the freshwater lens from seawater intrusion.

Study Area

Kish Island is located 19 km off the Iranian mainland in the Persian Gulf. Since the 1980s the island has been a free-trade zone and a highly popular holiday destination. It is currently estimated that about 1 million tourists visit the island annually (KFZO 2006). Kish is one of the few islands in the Persian Gulf with considerable fresh groundwater resources. In fact, until the midtwentieth century groundwater was the only source of freshwater for drinking and irrigation purposes in the island (Drees and Sommer 2004). However, due to the excessive exploitation of the groundwater resources in the past 3 decades, a constant decline in the groundwater quality has been reported by the native population. It is hard to quantify the level of groundwater deterioration given that no groundwater-monitoring system exists in the island and no widespread groundwater sampling has ever been performed prior to the current study. Based on field measurements conducted during this study, a freshwater lens with considerable areal extent still exists in the island, especially in the central and eastern parts. Groundwater in the western parts of the island is mostly saline. This part of the island has historically been less-developed (Ataie-Ashtiani et al. 2013a). Fig. 5 demonstrates the salinity contours of Kish Island based on field measurements of salinity in March 2010.

Table 2 illustrates some of the key characteristics of the study area adopted from Drees and Sommer (2004), KFZO (2006), and Ataie-Ashtiani et al. (2013a). Based on classifications of arid/semiarid/humid regions concerning both the mean annual precipitation [hyperarid, 0–50 mm; arid, 50–200 mm; semiarid, 200–500 mm; and humid, >500 mm (Lloyd 1986)] and the precipitation/evaporation ratio [arid, 0.5; semiarid, 0.5–1.0; and humid, >1.0 (Potter 1992)], the island is located in an arid environment. This means that a large percentage of the island’s modest rainfall is lost to evapotranspiration, resulting in an extremely fragile balance between the input and output components of the water budget (Kourakos and Mantoglou 2011).
To explore the subsurface geology of Kish Island, data from 62 previously drilled boreholes were gathered and analyzed. Based on this survey, the island’s geology mainly consists of two layers. The upper layer contains condensed sand along with traces of crushed coral and limestone shells. The thickness of this layer is approximately 17 m at the center of the island and decreases gradually towards the shore. The underlying layer is denser and less permeable and mainly consists of clay with lenses of silt (Ataie-Ashtiani et al. 2013a). The hydrogeological stratification of the model is applied by choosing different hydraulic conductivities for the two layers. Within each unit, the hydraulic conductivity is assumed to be isotropic in the vertical and horizontal directions.

Development of the Management Framework

Fig. 6 illustrates aerial photography of Kish Island. Based on similarities in land use and water consumption, the island’s surface is divided into 11 zones. Table 3 demonstrates the surface area and dominant form of land use in the proposed extraction zones.

The aim of the management model is to determine extraction rates for each of these 11 zones that would minimize seawater intrusion. Twenty observation wells (which were monitored during the research reported in this paper) are used to evaluate the extent of seawater intrusion in the simulation-optimization process. Fig. 7 shows the locations of the observation wells and the proposed extraction zones.

In the definition of sustainability, the choice of system boundary in time is crucial (Wheater et al. 2010). However, no predefined rule has been proposed for the selection of the planning period in a coastal aquifer-management problem. In the research reported in this paper, a 50-year planning period has been chosen based on the following motivations: (1) seawater intrusion is a slow phenomenon [and consequently it takes a number of years or decades for a management plan to show its effectiveness (Wheater et al. 2010)], and (2) a prolonged management period facilitates long-term planning of developments in the island. Feedback information from monitoring networks should be included in the methodology for sequential modifications.
As previously described, the initial simulations are based on the application of a variable-density groundwater numerical model. A number of simplifying assumptions are made, as follows:

(1) coastal marine boundary is assumed to be vertical and coastal slope is neglected, (2) fluctuations of the sea level are ignored, (3) solute and flow boundary conditions are presumed constant throughout the simulation period, (4) recharge is assumed to be uniform throughout the year (this assumption will not make a difference if the simulation period is in the magnitude of several years), and (5) a no-flow boundary with zero-concentration gradient is assumed at the bottom surface (at a depth of 500 m below the mean sea level). This depth is chosen based on a series of simulations with various depths to arrive at the minimum depth of simulation that does not affect the formation of salinity contours.

Fig. 8 illustrates the flow and solute boundary conditions. As demonstrated, a fixed concentration of 0.04 kg/kg is assigned to nodes that border the sea. This is a reasonable assumption due to the high salinity of Persian Gulf water (Ataie-Ashtiani et al. 2013a). The spatial discretization includes 18,000 nonuniform cubic elements with equal lengths of 500 m in the \( x \)-direction and \( y \)-direction (horizontal surface), and varying lengths of 2.19–27.11 m in the vertical direction.

Automatic calibration was performed based on total dissolved solid (TDS) values in 31 observation wells in November 2009. Fig. 9 demonstrates the spatial distribution of the observation wells. An assumption is made that the system is in equilibrium with respect to the current sea level. This is a widely used assumption, particularly when sufficient historic data for transient calibration is not available (Falkland 1991). A systematic parameter selection procedure was adapted for the selection of a small number of independent parameters for estimation, aimed at reducing parameter nonuniqueness and uncertainty in addition to the time spent on inverse-modeling computations. Eight parameters were initially selected for estimation, as follows: (1) hydraulic conductivity of the lower \( K_1 \) and upper \( K_2 \) layers, (2) transverse and longitudinal dispersivities \( \alpha_T \) and \( \alpha_L \), (3) porosity \( \varepsilon \), (4) recharge \( R \), (5) viscosity \( \mu \), and (6) molecular diffusion \( D_m \). Using the PEST inverse code, parameter sensitivities and overall correlations were subsequently calculated. From each pair of estimated parameters with a correlation coefficient close to 1 or −1, the parameter with the lower sensitivity was removed. The removed parameter was either assigned a fixed value based on desk studies or was tied to the other parameter with a fixed ratio. Within two PEST runs, the...
The number of variable parameters decreased from eight to two. The final set of independent parameters for automatic calibration include $K_1$ and $\alpha_L$, $R$, $\varepsilon$, and $D$ were given predetermined values in the final estimation attempt. $K_2$ and $\alpha_T$ appeared as dependent variables. $K_2$ was tied to $K_1$ with a factor of 10, and $\alpha_T$ was tied to $\alpha_L$ with a factor of 0.1. Table 4 demonstrates a summary of key parameter values in the calibrated model. Details of the calibration procedure are given in Ataie-Ashtiani et al. (2013a).

To render the optimization process computationally feasible, the numerical model is subsequently replaced by a trained ANN model as an approximate simulator. Determining the optimal ANN architecture involves the choice of how the information flows through the network and the selection of appropriate network geometry, denoting the number of layers and the number of neurons in each layer. Currently there is no unified approach for determination of an optimal ANN architecture. Only a few general guidelines are provided in the literature. A number of systematic approaches and rules-of-thumb have also been proposed but have failed to become the dominant method, most notably because they can easily be misused (Shahin et al. 2008). A comparative study was carried out to find the best combination of various ANN parameters. Different combinations of neurons were tested before arriving at the final architecture. Among the eight tested ANN models (Table 5), perceptron and back-propagation architectures have the worst performances. Feed-forward and linear filter neural networks display comparable performances. An increase in the number of hidden layers/neurons does not necessarily produce better results (Table 5). The number of neurons in the input and output layers are equal to the number of inputs and outputs, respectively. The number of neurons in the hidden layer is chosen based on best performance. Evaluations show that the architecture consisting of 11 input-layer neurons, 40 hidden-layer neurons, and 20 output-layer neurons with log-sigmoid transfer functions performs better compared to other architectures considered.

The training, testing, and validation patterns are generated using the calibrated SUTRA model. The ANN model is trained using input-output patterns of the net recharge rates and resulting salinity concentrations at selected observation locations using uniform distribution functions. Unfortunately, the long simulation-time required by the numerical model imposes a limit on the number of training sets that can be generated within a reasonable timeframe. In the research reported in this paper, a total of 56 data sets were produced by numerical simulations. The generated data sets have been randomly divided into three subsets, as follows: (1) 12 patterns are kept for testing, (2) 12 patterns for validation, and (3) the remaining 36 are used for training based on the cross-validation procedure (Stone 1974). Training is stopped when the error of the testing set starts to increase. The RMS error is the main criterion employed to evaluate the prediction performance of the ANN model. The output data have been scaled between 0.0 and 1.0 based on the fact that the log-sigmoid transfer function is being utilized. Table 6 illustrates the parameters related to ANN training, including best validation performance and coefficient of correlation $R$ values for the various sets. These variables form the basis for judgments on finding the best ANN architecture.

### Table 3: Surface Area and the Dominant Form of Land Use in the Proposed Extraction Zones

<table>
<thead>
<tr>
<th>Land usea</th>
<th>Surface area (km$^2$)</th>
<th>Area</th>
</tr>
</thead>
<tbody>
<tr>
<td>R</td>
<td>2.75</td>
<td>Zone 1</td>
</tr>
<tr>
<td>R</td>
<td>4</td>
<td>Zone 2</td>
</tr>
<tr>
<td>Mostly NP and R, eastern parts</td>
<td>11.5</td>
<td>Zone 3</td>
</tr>
<tr>
<td>Mostly R</td>
<td>6.25</td>
<td>Zone 4</td>
</tr>
<tr>
<td>R</td>
<td>2.75</td>
<td>Zone 5</td>
</tr>
<tr>
<td>R</td>
<td>5.5</td>
<td>Zone 6</td>
</tr>
<tr>
<td>AP and NP</td>
<td>16.25</td>
<td>Zone 7</td>
</tr>
<tr>
<td>NP, A, and R</td>
<td>10.5</td>
<td>Zone 8</td>
</tr>
<tr>
<td>NP, A, and R</td>
<td>13.5</td>
<td>Zone 9</td>
</tr>
<tr>
<td>NP, A, and R</td>
<td>7.25</td>
<td>Zone 10</td>
</tr>
<tr>
<td>NP, A, and R, northern parts</td>
<td>10.25</td>
<td>Zone 11</td>
</tr>
</tbody>
</table>

aA = arable land; AP = airport; NP = nonproductive land; and R = residential.
Linked Simulation Optimization

The ANN model is linked with GA in the framework of four multi-objective management models to identify the nondominated or Pareto-optimal solutions. Maximization of groundwater extraction and minimization of salinity in observation wells are equally significant. All four management models consider two conflicting objectives, as described in the following:

1. Minimization of total net recharge (natural and artificial recharge minus extraction) to the proposed extraction zones and hence maximization of total withdrawal from each zone. This objective can be represented as

\[
\min Z = \sum_{j=1}^{11} S_j \times n_j \quad j = 1, 2, \ldots, 11
\]

where \( Z \) = total net recharge to the island’s aquifer system (\( m^3/h \)), \( S_j \) = net recharge per surface area in the \( j \)th zone (\( m^3/m^2 \cdot h \)), and \( n_j \) = surface area of the \( j \)th zone (\( m^2 \)).

2. Minimization of seawater intrusion in the island’s freshwater lens. There are several possible representations of this objective. Therefore, as described in the subsequent paragraphs, in each of the four management models of the research reported in this paper, this objective is characterized in a unique form. In the first management model, the objective function is defined as minimization of the RMS change in TDS concentrations at the observation wells during the planning period. This objective function is aimed at keeping the concentration steady at every observation location over the time horizon. This objective function can be represented as

\[ F_7:1 \]

Fig. 7. Boundaries of the proposed extraction zones and the location of observation wells in the numerical model, subjected to spatial discretization

Fig. 8. Flow and solute boundary conditions
where \( C_{i,0} \) and \( C_{i,50} \) = TDS of the \( i \)th observation well at the start and end of the 50-year planning period (kg/kg), respectively.

In the second management model, adapted from Bhattacharjya and Datta (2009), the objective of minimizing seawater intrusion is characterized by minimization of the maximum TDS concentration in the observation locations. This objective function can be represented as

\[
\min \rightarrow \max C_{i,50} \quad i = 1, 2, \ldots, 20
\]  

In the third management model, the arithmetic mean of TDS concentration in the observation locations is minimized

\[
\min \rightarrow \sum_{i=0}^{20} C_{i,50} \quad 20
\]  

In the fourth management model, a trimmed arithmetic mean of TDS concentration in the observation locations is minimized.

\[
\min \rightarrow \frac{\sum_{i=0}^{20} C_{i,50}}{20}
\]
This trimmed arithmetic mean is obtained through the exclusion of 25% of the lowest and 25% of the highest TDS concentration in the observation wells

$$\min \rightarrow \frac{\sum_{i=5}^{15} C_{i,50}}{10}$$

All management models are subjected to positive values of total net recharge. Several factors need to be set when solving a problem with GA, including the population size, fitness, scaling, selection, crossover and mutation functions, and termination criteria. Table 7 illustrates parameter values employed in this procedure. In practice, the simulation-optimization procedure in the management models were terminated after the specified number of generations was reached.

### Discussion

Fig. 10 shows Pareto-optimal solutions for the four management models. The x-axis of diagrams (Fig. 10) represents the total net recharge to the island’s aquifer system. For a fixed natural recharge, any reduction in net recharge indicates that more groundwater can be extracted. Hence, minimization of the total net recharge results in the maximization of total withdrawal from the extraction wells for beneficial use. The y-axis of the diagrams (Fig. 10) represents the value of the objective functions corresponding to minimization of seawater intrusion. Regardless of the way the later objective

---

**Table 6. Parameters Related to ANN Training**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>T6:1 Best validation performance</td>
<td>0.00013 at 12 epochsa</td>
</tr>
<tr>
<td>T6:3 Regression analysis</td>
<td>R value for the training set 0.94</td>
</tr>
<tr>
<td>T6:5</td>
<td>R value for the validation set 0.82</td>
</tr>
<tr>
<td>T6:6</td>
<td>R value for the all data sets 0.88</td>
</tr>
</tbody>
</table>

Note: $R = $ coefficient of correlation.

aThe goal is to obtain a value of zero.

**Table 7. Parameters Used in the GA Optimization**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Scenario</th>
</tr>
</thead>
<tbody>
<tr>
<td>T7:2 Population size</td>
<td>165</td>
</tr>
<tr>
<td>T7:3 Creation function</td>
<td>Feasible population</td>
</tr>
<tr>
<td>T7:4 Selection function</td>
<td>Tournament</td>
</tr>
<tr>
<td>T7:5 Mutation function</td>
<td>Adaptive feasible</td>
</tr>
<tr>
<td>T7:6 Crossover function</td>
<td>Intermediate</td>
</tr>
<tr>
<td>T7:7 Stopping criteria</td>
<td>Generations 100</td>
</tr>
<tr>
<td>T7:8 Time limit</td>
<td>Infinite</td>
</tr>
<tr>
<td>T7:9 Fitness limit</td>
<td>Infinite</td>
</tr>
<tr>
<td>T7:10 Stall generations</td>
<td>50</td>
</tr>
<tr>
<td>T7:11 Stall time limit</td>
<td>Infinite</td>
</tr>
<tr>
<td>T7:12 Function tolerance</td>
<td>$1 \times 10^{-9}$</td>
</tr>
</tbody>
</table>

---

**Fig. 10.** Pareto-optimal solutions for the four management models: (a) management model (1); (b) management model (2); (c) management model (3); and (d) management model (4)
function is defined, the two objectives are inherently conflicting in all four management models. For any decrease in one of the objectives functions, an increase in the other objective can be observed (Fig. 10). Therefore, the optimal groundwater-extraction would be a compromise in some sense.

All diagrams (Fig. 10) show similar convex shape Pareto fronts with horizontal asymptotes. The horizontal asymptotes imply that the value of objective functions pertaining to the minimization of seawater intrusion (i.e., maximum TDS, root sum of squares of the change in TDS over the planning period, arithmetic mean of TDS, or trimmed arithmetic mean of TDS in the observation wells) remains fairly constant when the net recharge rate increase beyond a certain limit. This also indicates that as the quality of groundwater improves, further decrease in TDS concentrations would require exponentially more net recharge, resulting in an exponential decrease of permissible groundwater extraction.

The first management model, which seeks to maintain the current salinity distribution in the groundwater system through the prevention of further seawater intrusion, includes a very restrictive objective function [Fig. 10(a)]. This is apparent from the fact that using this objective, the permissible withdrawal from the study area is much smaller than that obtained using the other three management models. Moreover, there is no substantial variation in the Pareto-optimal values of the second objective function in the first and second management models [Figs. 10(a and b)]. This is essentially true for the second management model, in which the Pareto front covers a narrow range around TDS = 0.039 kg/kg. In the research reported in this paper, the TDS of Persian Gulf water surrounding Kish Island is assumed to be 0.04 kg/kg. The maximum TDS concentration in the second objective-function of this management model corresponds to an observation well near the shoreline, very close to the outer boundary of the transition zone between fresh and saline water. These locations are not much influenced by the net recharge rate within the intended limits and stay saline even if no groundwater is extracted. Based on the previous arguments, the first and second management-models are not very effective.

In the third management model, the minimization of seawater intrusion is represented by the minimization of the arithmetic mean of TDS concentration in the observation locations. As demonstrated by the Pareto front [Fig. 10(c)], this increases the effectiveness of the Pareto-optimal approach as larger variation in the Pareto-optimal values of the second objective are obtained. The effectiveness of the Pareto-optimal approach could be further enhanced by the exclusion of the lowest and highest TDS concentrations, which correspond to observation wells located either within the boundaries of the freshwater lens or close to the outer boundary of the transition zone between fresh and saline water. In both cases the TDS concentration is less influenced by the management model compared to wells located closer to the center of the transition zone. Since the location of the transition zone is a function of the recharge pattern, the relative position of the observation wells as compared to the transition zone cannot be determined in advance and the exclusion process cannot be performed prior to the linked simulation-optimization procedure.

The percentage variations in the Pareto-optimal values of the second objective-function in the four management models are 0.32, 0.1, 4.54, and 6.06%, respectively. Based on the previous discussion, the fourth management model seems to provide a more effective framework to incorporate the general objective of minimizing seawater intrusion while maximizing groundwater extraction.

A decision-maker can use the Pareto-optimal fronts (Fig. 10) to determine the amount of net recharge required to maintain the desirable quality of the water. Based on the Pareto-optimal solutions (particularly the position of the horizontal asymptotes and the change in the slope of the various Pareto front diagrams), a net recharge rate in the range of 150 and 250 m³/h (or 1.315 × 10⁶–2.190 × 10⁶ m³/year, which equals 7.3–12.1% of the total precipitation) would be a reasonable solution. Assuming a natural recharge rate of 20% (Drees and Sommer 2004), this choice would allow an extraction rate in the range of 2.304 × 10⁶ and 1.429 × 10⁶ m³/year. This rate should be divided among the previously defined extraction zones based on the results of the management model. To illustrate the possible outcome of the management model, the groundwater system has been simulated using the SUTRA numerical code for the 50-year planning period. This simulation is performed considering a total net recharge of 2.18 × 10⁶ m³/year (reasonably selected from the Pareto front diagram) distributed among the defined extraction zones in accordance with the results of the fourth management model.

This choice would allow for 1.44 × 10⁶ m³/year of groundwater extraction from the island freshwater lens. Fig. 11 illustrates the resulting 3D view of the simulated salinity contour map of Kish Island. Fig. 11 also presents the salinity contour map of the calibrated model to illustrate the salinity conditions at the start of the planning period. Fig. 12 shows the net recharge and permissible extraction rate from extraction zones based on the exemplar proposed management.

**Fig. 11.** Three-dimensional view of simulated salinity contour map of Kish Island, (a) using the calibrated model to represent conditions at the start of the planning period, and (b) conditions at the end of the 50 year planning period if the exemplar management model is employed.
Fig. 12. Schematic distribution of the net recharge and permissible extraction rates for managerial zones based on the exemplar model.

Fig. 13. Schematic representation of salinity variations in the observation wells between the start and end of the 50-year planning period based on the exemplar management model.

Conclusion

Optimal management of groundwater extraction in coastal aquifers has been a challenging subject of numerous studies in the past, but most studies have been limited to hypothetical examples and few have focused on field problems, especially in small islands with entity complexities (e.g., Banerjee et al. 2011). There is a lack of literature on simulation-optimization approaches to coastal aquifer-management problems in real-world applications. The current scientific challenges of coastal aquifer management in the real-world are as difficult and diverse as the systems themselves. Considering the limited and highly stressed nature of fresh groundwater in many small islands around the world, characterizing and managing such coastal aquifers are particularly a major scientific and significant challenge.

This paper shows that integration of the latest innovative tools can provide the means to solve complex real-world optimization problems in an effective way and that application of simulation-optimization paradigms can be effectively extended to large-scale field applications. Computational time has long been considered a major complication in applying the linked simulation-optimization procedure to field problems. A way around this problem is to...
use surrogate models based on ANNs in linked simulation-optimization models for solving the groundwater-management problems. A number of recent studies have also used GP in a similar approach (e.g., Sreekanth and Datta 2011).

In the research reported in this paper, a 3D density-dependent numerical model was replaced by an ANN model with one hidden layer. Consequently, the amount of computational resources spent on simulation was strictly reduced. Results indicate that even with a moderate number of input data sets based on numerical simulations, the ANN metamodel can be effectively trained. This is vital to the computational feasibility of the procedure if complex density-dependent numerical models are to be employed. The limited performance-evaluation results show that the developed methodology is potentially applicable to solving multiobjective groundwater-extraction management problems in small islands and other coastal aquifer systems. The introduction of extraction zones in the research reported in this paper provides a high degree of flexibility in the choice of management models and implementation of the proposed plan. For similar studies in the future, the authors recommend that extraction zones be used in regional-scale cases instead of point-well locations. Surrogate models of seawater intrusion based on GP could also be a possibility for advancement in future research.

Acknowledgments

The research reported in this paper was supported under grant number 17/419295 by the Iran Kish Free-Zone Organization. The writers are grateful for the constructive comments of the editor and two anonymous reviewers, which helped improve the final paper.

Notation

The following symbols are used in this paper:

- $a$ = number of nodes in the input layer of the ANN;
- $b$ = number of nodes in the hidden layer of the ANN;
- $b_i$ = vector of the $i$th simulation results in the SUTRA formulation;
- $b_j$ = bias of the $j$th node in the present layer of the ANN;
- $C_{i,0}$ = TDS of the $i$th observation well at the start of the 50-year planning period;
- $C_{i,50}$ = TDS of the $i$th observation well at the end of the 50-year planning period;
- $C_r$ = recharge water concentration;
- $C_s$ = seawater concentration;
- $c^*$ = concentration of solute in the source fluid;
- $D$ = mechanical dispersion tensor;
- $D_m$ = apparent molecular diffusion coefficient;
- $f$ = activation function in the present layer of the ANN;
- $g$ = gravitational acceleration;
- $H_i$ = $i$th nodal value in the hidden layer of the ANN;
- $I = n \times n$ = identity tensor in the SUTRA formulation;
- $J = Jacobian matrix in the SUTRA formulation;
- $J_{ij} = $ derivative of the $i$th observation with respect to the $j$th parameter in the SUTRA formulation;
- $K_1$ = lower-layer hydraulic conductivity;
- $K_2$ = upper-layer hydraulic conductivity;
- $k$ = solid matrix permeability;
- $m$ = number of monitoring/observation wells;
- $N$ = number of nodes in the previous layer of the ANN;
- $n$ = number of extraction zones;
- $n_j$ = surface area of the $j$th zone;
- $o$ = number of nodes in the output layer of the ANN;
- $p$ = fluid pressure;
- $Q_s$ = fluid mass sink or source;
- $R$ = recharge (natural or artificial);
- $r$ = vector of residuals for the current parameter set in the SUTRA formulation;
- $S_n$ = net recharge per surface area in the $j$th zone;
- $S_{np}$ = specific pressure;
- $T$ = transpose matrix;
- $t$ = time;
- $v$ = average fluid velocity;
- $w_{ij}$ = observation weight in the SUTRA formulation;
- $w_{ji}$ = weight connecting $x_i$ and $y_j$ (ANN model);
- $X_i$ = $i$th nodal value in the input layer of the ANN;
- $x_i$ = $i$th nodal value in the previous layer of the ANN;
- $x_j$ = $j$th parameter in the SUTRA formulation;
- $Y_j$ = $j$th nodal value in the output layer of the ANN;
- $y_j$ = $j$th nodal value in the present layer of the ANN;
- $Z$ = total net recharge (recharge minus extraction);
- $\alpha$ = Marquardt parameter in the SUTRA formulation;
- $\alpha_f$ = longitudinal dispersivity;
- $\alpha_T$ = transverse dispersivity;
- $\varepsilon$ = aquifer volumetric porosity;
- $\mu$ = fluid dynamic viscosity;
- $\mu_f$ = dynamic viscosity of fresh water;
- $\rho$ = fluid density.
- $\phi$ = optimal parameter set for which the sum of the squared deviations between the model-generated observations and experimental observations is reduced to a minimum in the SUTRA formulation; and
- $\Omega$ = number of observations in the SUTRA formulation;

References


