

Predicting Conductance Due to Upconing Using Neural Networks

by Emery A. Coppola Jr.¹, Charles F. McLane², Mary M. Poulton³, Ferenc Szidarovszky⁴, and Robin D. Magelky²

Abstract

Artificial neural networks (ANNs) were developed to accurately predict highly time-variable specific conductance values in an unconfined coastal aquifer. Conductance values in the fresh water lens aquifer change in response to vertical displacements of the brackish zone and fresh water–salt water interface, which are caused by variable pumping and climate conditions. Unlike physical-based models, which require hydrologic parameter inputs, such as horizontal and vertical hydraulic conductivities, porosity, and fluid densities, ANNs can “learn” system behavior from easily measurable variables. In this study, the ANN input predictor variables were initial conductance, total precipitation, mean daily temperature, and total pumping extraction. The ANNs were used to predict salinity (specific conductance) at a single monitoring well located near a high-capacity municipal-supply well over time periods ranging from 30 d to several years. Model accuracy was compared against both measured/interpolated values and predictions were made with linear regression, and in general, excellent prediction accuracy was achieved. For example, although the average percent change of conductance over 90-d periods was 39%, the absolute mean prediction error achieved with the ANN was only 1.1%. The ANNs were also used to conduct a sensitivity analysis that quantified the importance of each of the four predictor variables on final conductance values, providing valuable insights into the dynamics of the system. The results demonstrate that the ANN technology can serve as a powerful and accurate prediction and management tool, minimizing degradation of ground water quality to the extent possible by identifying appropriate pumping policies under variable and/or changing climate conditions.

Introduction

Effective ground water management often requires models that can accurately predict system responses under spatially and temporally variable conditions like weather and pumping. In coastal areas where population is increasing rapidly, a critical ground water management issue is degradation of water quality due to salt water upconing and/or intrusion. These phenomena are caused

primarily by excessive ground water pumping withdrawals, which change the natural dynamic equilibrium between the fresh water–salt water interface, allowing salt water containing high concentrations of dissolved ions to migrate upward and/or inland, contaminating portions of the fresh ground water supply.

Accurate prediction and management models can delay if not eliminate the need for expensive mitigation measures and may even prevent loss of an irreplaceable ground water resource. There are, however, significant challenges in developing a ground water model with limited field data that is capable of making accurate predictions in both space and time (Anderson and Woessner 1992; Coppola et al. 2003b). Typically, modeling the physical flow conditions of a real world ground water system is inherently difficult because of the complexity and variability of natural systems (Gelhar 1993). Modeling and accurately predicting movement of the brackish zone and fresh water–salt water interface can be even

¹Corresponding author: NOAH LLC., 610 Lawrence Road, Lawrenceville, NJ 08648; (609) 434-0400; emerynoah@comcast.net

²McLane Environmental LLC., 707 Alexander Road, Suite 206, Princeton, NJ 08540-6331.

³Department of Mining and Geological Engineering, University of Arizona, Tucson, AZ 85721-0012.

⁴Department of Systems and Industrial Engineering, University of Arizona, Tucson, AZ 85721-0020.

Received May 2004, accepted January 2005.

Copyright © 2005 National Ground Water Association.

doi: 10.1111/j.1745-6584.2005.00092.x

more difficult. Concentration and density gradients and microscale phenomena like molecular diffusion, which often have significant effects on local water quality conditions, are difficult and expensive to field characterize, thereby constraining efforts to accurately simulate the transport phenomena with a physical-based model (Voss and Souza 1987).

As an alternative “learning” modeling paradigm, artificial neural networks (ANNs) do not require explicit representation of the physical laws and conditions governing the system behavior of interest. For predicting conductance values at the single monitoring well for this problem, the ANNs do not simulate advective and dispersive processes with physical-based equations. Instead, the ANN obtains a complex mathematical relationship that predicts outputs, constituting the system behavior of interest, in response to predictor input variables. This functional mapping is done in a manner analogous to human learning, where observation data is processed through an interconnected network of nodes in an effort to learn relationships between cause and effect variables. Thus, for this ground water quality prediction problem, the need to represent relatively complex processes with physical-based equations as well as quantify aquifer properties and boundary conditions, many of which may be highly variable over space and/or time, is virtually eliminated.

In the earliest ANN-related ground water modeling, ANNs were trained with numerical model simulation data. In one of the first ANN-ground water modeling applications, Rogers and Dowla (1994) trained an ANN with a numerical contaminant transport model to estimate several objective function values (e.g., remediation cost), from which the optimal pumping and injection system for remediating a ground water contaminant plume was identified. Coppola (2000) and Coppola et al. (2003b), using MODFLOW simulation data, developed ANNs that accurately predicted transient ground water levels at locations of interest in response to variable pumping and recharge conditions; the ANN-derived state-transition equations constituted the basis of a multiobjective optimization analysis for a wellfield in proximity to a contaminant plume. Gumrah et al. (2000) trained an ANN with computer simulation data to predict both water levels and chloride concentrations in a hypothetical confined aquifer due to well injection of brine through a single well. Rao et al. (2003) developed an ANN simulator from the SHARP interface model to optimize pumping strategies that minimize excessive salt water intrusion. In more recent ground water applications, ANNs have been developed with real world data. Coulibaly et al. (2001) trained ANNs to estimate water-level changes in an unconfined aquifer in response to variable weather conditions. Coppola et al. (2003a, 2003b, 2005) present various case studies where ANNs were developed with real world data for accurately predicting transient ground water levels under variable weather and pumping conditions in different types of ground water systems.

The purpose of this study was to determine whether ANNs could be developed with real world data to accurately predict transient and highly dynamic ground water quality conditions in response to variable weather and

pumping conditions. The capability of ANN technology to accurately reproduce water quality changes in the vicinity of a municipal supply is compared against measured/interpolated values and multivariable linear regression (LR). In addition, the ANNs were used to conduct sensitivity analyses, and the results are assessed for validity within the context of the physical system dynamics. Because of a lack of basic data and uncertainty with existing data, accurate development and calibration of a three-dimensional (3D) numerical solute transport model for comparison was not attempted for this site. This reinforces one of the inherent strengths of the ANN approach that such difficult-to-collect, uncertain data (e.g., 3D distribution of saline water, aquifer transmissivity, etc.) are not required as model inputs.

Finally, although not demonstrated in this study, one of the great benefits offered by ANN technology is its high computational speed, so that model output can be obtained nearly instantaneously. In addition, unlike traditional physical-based models, it can be integrated directly with continuous real-time data streams (e.g., SCADA). The ANN predictive accuracy can be further improved by initializing the model to real-time conditions. Thus, the combination of its high computational speed, high predictive accuracy, and direct linkage with an on-line data collection and control system [e.g., Supervisory Control and Data Acquisition (SCADA)] makes it possible to quickly compute accurate management decisions that reflect real-time conditions.

ANN Background

Coppola et al. (2005) provide an overview of basic ANN concepts related to architecture, transfer functions, learning algorithms, development heuristics, and issues related to ground water modeling. For convenience, however, a relatively brief overview of ANN architecture, transfer functions, and some theoretical justification is presented here, but the interested reader is referred to the two-part series from the ASCE Task Committee on Application of Artificial Neural Networks in Hydrology (2000a, 2000b).

Figure 1 depicts a simple architecture example for the most commonly used ANN paradigm, the multilayered perceptron, which was also used in this study. The ANN architecture in this case consists of three distinct layers: an input, hidden, and output layer, each consisting of individual nodes that are fully interconnected with nodes in the adjacent layer. Except for the single bias node, which helps provide numerical stability, individual nodes in the input layer represent the input variables for the problem, and the nodes in the output layer represent the output variables that the ANN is trying to predict.

Connections between the nodes consist of a mathematical function, called a transfer (or squashing) function, which can be linear or nonlinear in form. In this study, the commonly used nonlinear hyperbolic transfer function was selected. The transfer function is expressed in terms of the nodal input values and connection weights that link each node.

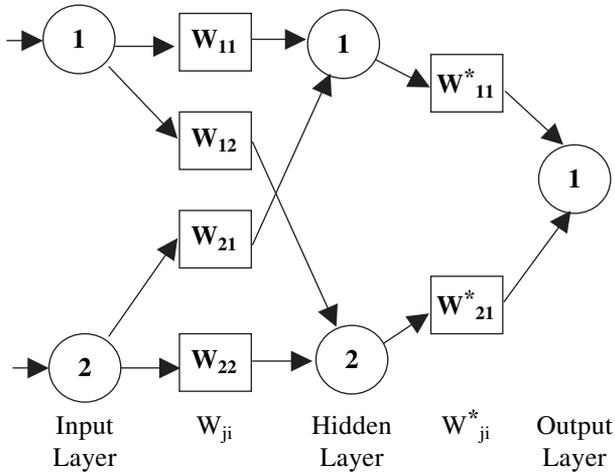


Figure 1. A simple architecture example depicting the multilayered ANN perceptron, consisting of input, hidden, and output layers, with weight connections between interconnected nodes.

In this work, the commonly employed nonlinear hyperbolic tangent transfer function

$$f_j(\text{Sum}_j) = \frac{e^{\text{Sum}_j} - e^{-\text{Sum}_j}}{e^{\text{Sum}_j} + e^{-\text{Sum}_j}} \quad (1)$$

was used, where Sum_j represents the weighted sum for a node in the hidden layer, and e denotes the basis of the natural logarithm. In Sum_j , the input value received by each node in the hidden layer is multiplied by an associated connection weight, whose value is identified during learning. This weighted sum can be formally represented as

$$\text{Sum}_j = \sum_{i=1}^n w_{ji}x_i + w_{jb} \quad (2)$$

where w_{ji} represents the connection weight between the i th node in the input layer and the j th node in the hidden layer. The input x_i is known and represents the values of the input variables for node i in the input layer. A bias unit, which helps to provide numerical stability, is merely added as the connection weight w_{jb} because it has a constant input value of 1.0.

There are various kinds of learning algorithms, including back-propagation and conjugate gradient. During learning, the ANN processes training patterns consisting of input-output patterns through the network, systematically adjusting the connection weights, so that the measure of the overall goodness of the ANN model defined as the root mean squared error (RMSE) between the ANN-estimated output values and the actual values is minimized.

The RMSE is mathematically defined as:

$$\text{RMSE} = \sqrt{\frac{1}{N} \sum_{k=1}^N (\gamma_k - C_k)^2} \quad (3)$$

where γ_k is the ANN-estimated conductance value for the k th training event, C_k is its corresponding measured/interpolated value, and N denotes the total number of such events.

ANNs are often compared to regression in the sense that both use empirical-based equations to map a set of input variables to a set of output variables. However, the interconnected structure of the ANN architecture as well as the functional form of the transfer functions endow it with special mathematical and modeling properties that exceed the power of regression. From a purely mathematical perspective, what separates ANNs from regression is Kolmogorov's theorem, which guarantees that any continuous function with n variables can be exactly represented by a three-layered ANN consisting of n inputs and $2n+1$ hidden nodes. From a modeling perspective, unlike regression, which treats each output variable independent of the other, the ANN architecture allows capture of the interrelationship or interdependency that often exists between output variables and hence may further increase predictive capability.

Study Area

The study area is located within the Pamet Lens, a fresh water lens aquifer, on the northern tip of the Cape Cod, Massachusetts peninsula. Figure 2 depicts the general study area with both a regional and local cross-sectional view, including well locations relative to each other and the fresh water/salt water interface. Glacial outwash deposits, consisting primarily of sand and gravel interbedded with silt and clay, overlie a low permeability bedrock formation that is estimated to exist at a depth of ~120 m below mean sea level (msl) at the site (Oldale 1969). The shallow unconfined aquifer is formed by a thin fresh water lens floating on a denser body of salt water, which extends into the bedrock formation. Hydraulic conductivity for the shallow production zone ranges from 30 to 140 m/d with a representative specific yield value estimated at ~0.25 (Masterson 2004; Guswa and LeBlanc 1985; Cape Cod Planning and Economic Development Commission 1989; Camp Dresser & McKee Inc. [CDM] 1985).

Following contamination of a major nearby wellfield by a leaking underground storage tank in the late 1970s, a temporary municipal well, Test Site No. 4 Production Well (TSN4), was installed to supply drinking water. Pumping of TSN4 from the late 1970s to mid 1980s resulted in salt water upconing in the fresh water lens. Seasonal water quality changes due to upconing were monitored over time by the USGS with periodic conductance-level measurements in the nearby observation well TSW-235. Eventually, the production well was taken out of service and the petroleum-impacted wellfield was brought back on line. Although the TSN4 well is no longer in use, similar wells in the area are at risk to salt water upconing, and local water purveyors are pursuing appropriate management tools and strategies, which motivated this current ANN model development study.

The prepumping equilibrium water table elevation at TSN4 was ~1.3 m above msl in 1978. Water quality data collected in the fall of 1979 from observation wells at various depths delineated a gradual 15-m brackish

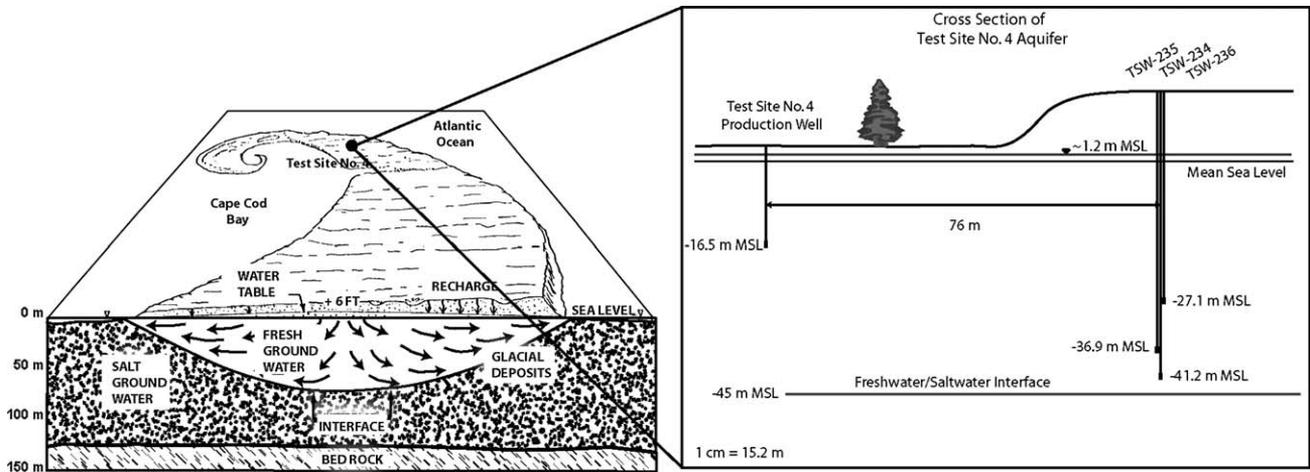


Figure 2. The study area and aquifer cross section in both regional and local view.

transition zone with a midpoint depth of ~ 45.1 m below msl, ~ 8 m below observation well TSW-235 (the focus of ANN modeling in this study), and 29 m below production well TSN4 (Figure 2). The average thickness of the fresh water aquifer in the vicinity of the well is ~ 46.3 m.

Fresh water chloride concentrations near the site ranged from 31 to 36 ppm, while salt water chloride concentration was $\sim 16,000$ ppm. Sodium concentrations (assuming sodium content to be $\sim 55\%$ of chloride content) ranged from ~ 17 to 20 ppm in the fresh water zone and averaged ~ 8800 ppm in the underlying salt water. To provide context for these values and the measured and simulated values reported subsequently, as well as underscore the importance of preventing excessive upward migration of the fresh water–salt water interface, the federal drinking water standard for total dissolved solids is 500 ppm, the secondary standard for chloride is 250 ppm, and the health guideline for sodium is 20 ppm.

ANN Architecture and Data

Separate ANNs were trained and validated for 30-, 60-, and 90-d prediction periods to examine system response for wellfield management horizons ranging from a peak production month through an entire 3-month summer season. If necessary, ANNs could be developed for longer planning horizons, as is demonstrated later in the paper, to assess the impact of the ground water system under changing pumping and climate conditions and to formulate appropriate longer-term management policies.

The four predictor variables used in this study are listed subsequently and are consistent with previous ground water-level prediction work conducted by Coppola et al. (2003a, 2003b, 2005):

1. Initial conductance value measured/interpolated at beginning of prediction period
2. Mean daily temperature measured over the prediction period
3. Total precipitation measured over the prediction period
4. Total ground water pumping extraction over the prediction period.

For this ANN application, the initial system state, conductance, as measured at the beginning of the prediction period, is combined with predictor variables that implicitly represent a mass balance approach. With this approach, a potential source term, precipitation, is used in conjunction with two potential sink terms, temperature, which serves a surrogate variable for both soil-moisture deficit and evapotranspiration, and pumping extraction. Cumulatively, these source and sink terms capture the differential changes in aquifer storage that influence the elevation of the water table, and concomitantly, movement of the brackish zone, which largely determines the final measured conductance level. The single ANN output variable is final conductance (measured in $\mu\text{S}/\text{cm}$) in observation well TSW-235 at the conclusion of the prediction period (i.e., event).

All three ANNs consisted of a three-layered perceptron architecture, with four input variable nodes and a single bias unit, six hidden-layer nodes, and one output node (Figure 3). A combination of back-propagation and

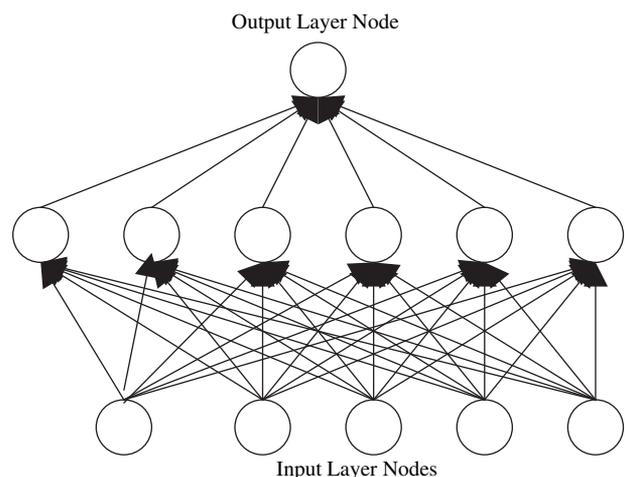


Figure 3. Three-layered ANN perceptron architecture used in study: four input nodes and single bias node in input layer, six hidden nodes, and one output node. Input variables are initial conductance, total precipitation, mean daily temperature, and total ground water pumping extraction; output variable is final conductance.

conjugate gradient learning algorithms were used for learning.

The daily data set used for ANN development and validation spanned the period from June 1, 1981, to January 31, 1985. Historical temperature and precipitation data were obtained from the National Oceanic and Atmospheric Administration for a nearby weather station (Provincetown, Massachusetts). As discussed previously, conductance data was collected by the USGS. There were some data gaps, where daily values for temperature and/or precipitation were not available. However, there was sufficient sequential data to generate adequate data sets for training and validating the ANNs. Conductance values were typically measured once every 1 to 2 months. In order to interpolate missing daily data values, a cubic spline method (Yakowitz and Szidarovszky 1989) was used to approximate conductance values between measuring points to provide daily data for ANN development and validation.

A moving average approach was used to generate ANN data sets. That is, each successive ANN data pattern, consisting of the four ANN inputs and the single output, was offset by 1 d from the previous pattern. For example, for the 30-d prediction period, if the first pattern used data beginning June 1, 1980, all subsequent days through June 30, 1980, were used for computing the values of the ANN variables. Thus, the mean daily temperature, total precipitation, and total ground water pumping withdrawals used daily values for all days from June 1 through June 30, with the final conductance value measured/interpolated on June 30 serving as the "target" prediction value. For the next training pattern, the data, offset by 1 d from the previous pattern, began June 2, 1980, and terminated July 1, 1980. The same approach was used for the 60- and 90-d prediction periods as well. This moving average approach provided sufficiently large data sets, despite climate data set discontinuities and the relatively long prediction horizons.

ANN Development

ANN training and validation data sets should span the observed or expected range of system behavior to ensure that the ANN has the opportunity to "learn" the expected range of system behavior. Similarly, during validation, care should be taken to determine whether the ANN has learned system behavior of interest over the

range of expected conditions, so that the user (in this case a wellfield operator) can be confident that the ANN can provide predictions with an acceptable level of accuracy. In situations where the system possibly exceeds the extreme range of behavior for which the ANN was trained, the user must carefully exercise judgment in assessing predictive capability. One of the limitations of the ANN approach is that, in general, it does not accurately extrapolate far outside the range over which it has been trained with. However, this limitation could possibly be addressed by generating synthetic data sets with a physical model that simulates extreme conditions not yet measured or encountered. These extreme event simulation data sets could be combined with available real world data to train the ANN and extend its predictive capability. The other options are to rely on a physical-based model, expert judgment, or some combination thereof, while re-training the ANN with new extreme data as it becomes available.

During ANN development, learning proceeds in a series of training and verification steps. The ANN is presented with training data during which patterns are processed through the network, and the learning algorithm adaptively adjusts the network connection weights to minimize the RMSE between actual and estimated output values. Intermittently, the training phase is interrupted, and a separate (verification) data set is processed through the ANN to verify progressive learning, as indicated by a declining RMSE value obtained with the verification data set. Verification guards against overtraining, where the ANN has memorized or overfitted the connection weights to the training patterns. Training proceeds until the verification RMSE either stabilizes or begins to increase. At this point, ANN training is terminated, and the ANN can now be validated with a third data set not previously used for training or verification.

To provide robust training, verification, and validation, statistically similar data sets spanning the expected range of system behavior were used for ANN development and validation. Note that each of these three data sets include measurements spanning the entire period of data, and thus are not restricted to only certain segments of time. Table 1 presents a summary of the number of data patterns used for training, verifying, and validating each ANN, with a statistical summary of the final ANN conductance values for each prediction period. The minimum and maximum values are presented to emphasize

Table 1
Summary of ANN Data Sets

Days	No. of Patterns for Training	No. of Patterns for Verification	No. of Patterns for Validation	Total No. of Patterns	Minimum Final Conductance Value	Mean Final Conductance Value	Maximum Final Conductance Value
30	338	159	165	662	595.0	2362.4	4004
60	241	120	120	481	796.4	2517.5	4004
90	180	90	92	362	1692.1	2607.3	4004

Note: Conductance measured in units of $\mu\text{S}/\text{cm}$.

that conductance did exhibit relatively large temporal changes over the prediction periods of interest, and thus the aquifer as it pertains to this water quality condition is a fairly dynamic system.

As the table shows, approximately half the number of patterns used for ANN training was used for verification, with the same ratio applying to validation. Also, the minimum, mean, and maximum conductance values are similar for the three data sets, with the exception of the minimum value for the 90-d prediction period. This inconsistency is due to data gaps; because n consecutive days of complete daily data are required to generate an n -d prediction event, there is more chance of an incomplete data set (i.e., missing day of precipitation) for the longer prediction periods (i.e., 60 and 90 d). In this case, the lower conductance values did not fall within a complete consecutive daily data set required for the 60- and 90-d prediction periods.

ANN Prediction Results

Table 2 summarizes the overall ANN prediction performance for all data (i.e., training, verification, and validation) for the three prediction periods within the context of observed changes. For example, for all 90-d prediction period events, the computed absolute mean change of conductance is 885.9 $\mu\text{S/cm}$, while the mean absolute ANN prediction error is only 25.4 $\mu\text{S/cm}$. The maximum conductance-level change for any single 90-d period was 1765.1 $\mu\text{S/cm}$, while the maximum discrepancy between any single ANN prediction and its corresponding measured/interpolated value was just 97.7 $\mu\text{S/cm}$.

Figure 4 depicts the measured/interpolated conductance values against the ANN-predicted values for the 30-, 60-, and 90-d prediction horizons for every third data point. The figure demonstrates the high accuracy achieved with the ANNs for the three prediction periods, despite relatively large changes in conductance levels per prediction period. Thus, the relatively low ANN prediction errors would help an operator maintain conductance within a narrow range of desired levels with high reliability. Note that no distinction between training, verification, and validation points is made, as the ANN errors for all three data sets were almost identical.

The finding that ANN accuracy was best for the 90-d period seems counterintuitive until one further analyzes

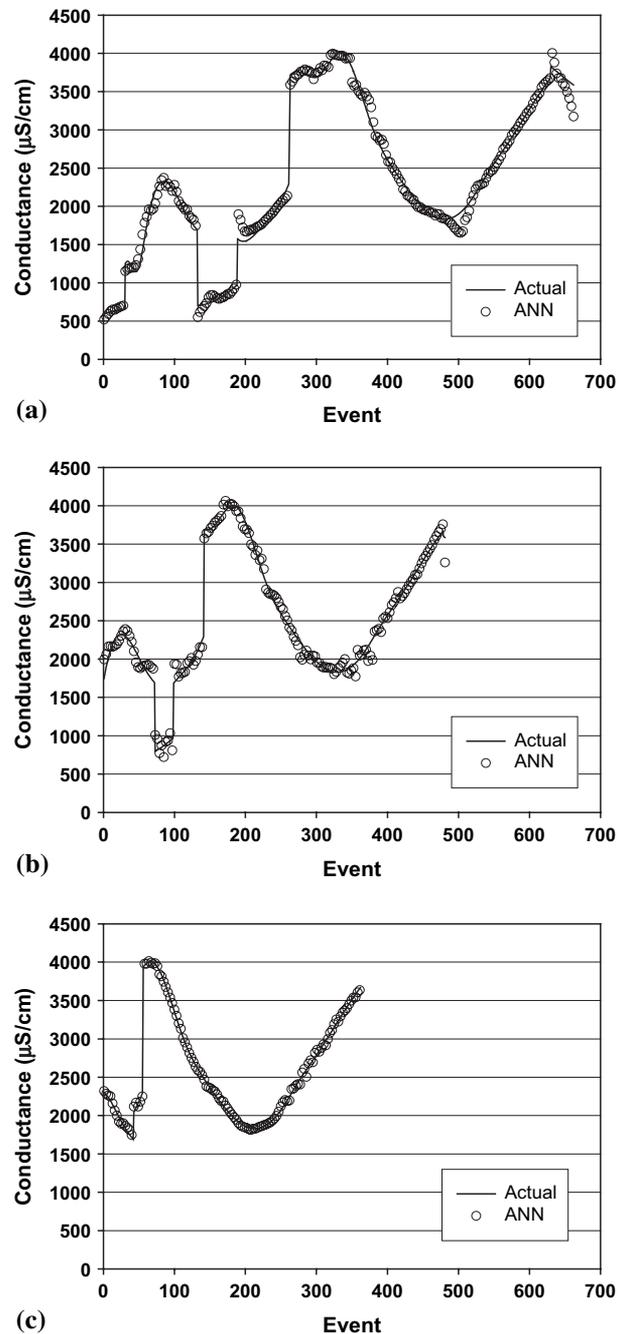


Figure 4. ANN vs. measured/interpolated conductance values for the (a) 30-d prediction period, (b) 60-d prediction period, and (c) 90-d prediction period.

Table 2 Statistical Summary of ANN Predictive Performance for All Data			
Statistical Measure Final Conductance	30-d Period	60-d Period	90-d Period
Absolute mean change	308.7	612.3	885.9
Maximum change	1110.6	1360.3	1765.1
Absolute mean prediction error	61.8	67.6	25.4
Maximum prediction error	414.5	327.0	97.7

Note: Units are in $\mu\text{S/cm}$.

the relationships between the input variables with the output variable over different time periods. As will be discussed in more detail later in ANN Sensitivity Analysis, the physical dynamics of the system apparently result in greater correlation between individual input predictor variables (i.e., temperature) and conductance over the 90-d prediction periods, yielding superior ANN performance.

ANN vs. Linear Regression

As a benchmark for ANN performance, LR was also conducted on the same data sets with the identical input

Table 3
Mean Absolute Error Achieved with ANN and LR for All Data

Prediction Period (d)	ANN	LR
30	61.8	148.5
60	67.6	168.9
90	25.4	99.7

Note: Units are in $\mu\text{S}/\text{cm}$.

and output variables. A comparison in predictive accuracy between the two methods is shown in Table 3.

While LR had an absolute mean error that was on average 2 to 4 times higher than that achieved with ANN, it still performed very well in relation to the large changes in conductance. As with the ANN approach, the predictive capability of LR generally increased for longer prediction periods, as correlation between inputs and final conductance became stronger. Figure 5 compares ANN against LR (plotting only every third data point for clarity) for the 90-d prediction period, where the discrepancy between the two methods was highest.

ANN Sensitivity Analysis

Two types of sensitivity analyses were used to assess the interrelationships between the input predictor variables and the output variable conductance, and to foster a deeper and more complete understanding of aquifer system behavior.

The first set of sensitivity analysis results obtained from the validation data are presented in Table 4 for the 30-, 60-, and 90-d prediction periods. Training sensitivity RMSE ratios were similar in value and generated identical rankings, confirming the sensitivity characteristics of the system depicted in Table 4.

The sensitivity analyses quantify and rank the importance of each of the four input variables by examining the change in RMSE if the particular input variable is eliminated. For example, for the 30-d prediction period,

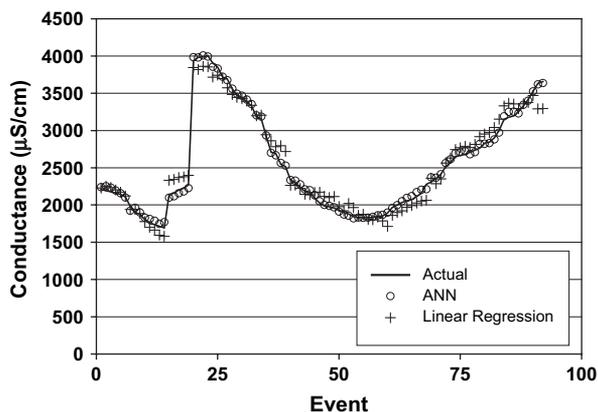


Figure 5. ANN and LR vs. measured/interpolated conductance values for the 90-d prediction period.

eliminating the total monthly precipitation input variable nominally increases the RMSE for the validation data set by a factor of 1.3 (i.e., RMSE ratio), which ranks this predictor variable as the least important (4); in comparison, eliminating the initial conductance input variable increases the RMSE during validation by a factor of 13.3, ranking this variable as the most important predictor (i.e., rank 1).

The relative importance (ranking) of the four prediction variables remains the same for all three prediction periods. Generally, all four predictor variables become significantly more important for accurately predicting final conductance levels over the 90-d prediction period, as reflected by the increasing RMSE ratio values. For the three source/sink terms (i.e., precipitation, temperature, and pumping extraction), this is likely due to an increased correlation between these variables and conductance levels over longer periods. For example, during the summer season, characterized by higher temperatures, pumping extraction increases to meet greater consumer demand, increasing conductance levels. There is a natural temporal correlation, therefore, between temperature and pumping extraction, which becomes stronger over 90-d periods, and both variables correlate strongly with conductance levels. In addition to correlating with pumping extraction, temperature also strongly influences evapotranspiration rates and soil-moisture deficits, which, in combination with precipitation, determine recharge rates. Recharge rates affect ground water levels, which in turn influence conductance levels. Over the longer 90-d prediction period, precipitation or lack thereof has a larger effect on the ground water levels, again influencing conductance levels. By contrast, over relatively shorter periods, precipitation is not expected to have as much of an effect on ground water levels due to the relatively high specific yield value (0.25) of the aquifer. There is likely some correlation between precipitation and pumping extraction, but over the relatively long time periods considered, it does not appear to be important. Collectively, the three source/sink variables have an implicit relationship with ground water-level changes which, in accordance with the well-known Ghyben-Herzberg relation, induces vertical displacements of the brackish zone and fresh water-salt water interface, which changes conductance levels.

In a second sensitivity analysis, only the initial conductance and total ground water extraction were used as inputs to the ANNs for predicting final conductance values to examine ANN performance for the case where daily climate data may not be available. A similar analysis was conducted using LR. Table 5 compares the results obtained with the two methods for the three prediction periods both with and without the climate input variables precipitation and temperature.

As expected, without climate inputs, the prediction performance of both methods declined, and the ANN continued to outperform LR, particularly for the 90-d prediction period. Figure 6 compares ANN and LR predictions (every third point) against measured/interpolated conductance values for the 90-d prediction horizons without climate inputs.

The prediction errors for the ANN models that included the climate inputs (i.e., temperature and

Table 4
Sensitivity Matrix for ANN Prediction Periods (Validation Data set)

	Initial Conductance	Total Ground Water Extraction	Mean Temperature	Total Precipitation
Importance rank	1	2	3	4
30-d RMSE ratio	13.3	5.8	3.6	1.3
60-d RMSE ratio	10.2	5.1	2.7	2.1
90-d RMSE ratio	25.5	17.6	14.4	4.9

Note: Units are in $\mu\text{S}/\text{cm}$.

precipitation) are approximately 1/3 to 1/2 of the error achieved with the ANN models that did not use these inputs. As with predictions made with climate inputs, ANN predictions made without climate inputs improved over longer prediction periods. Because pumping extraction is strongly correlated with temperature, particularly over longer time periods, and precipitation is the least important predictor variable, the relatively high prediction accuracy achieved without climate inputs is consistent. Still, the results demonstrate that because climate conditions do affect movement of the brackish/saline zone in the short term, they should be used when possible to increase system understanding through sensitivity analysis and improve management decisions via superior predictive capability.

Multiple-Year Prediction Horizon Using Monthly Stress Periods

In the work presented previously, three ANNs were trained to predict final conductance values at 30-, 60-, and 90-d prediction period horizons. In this section, the previously presented ANN and LR models developed for predicting conductance levels 30 d into the future were used to forecast the end of month conductance values over a multiple-year horizon from June 1981 through January 1985. During portions of this time period for which measured conductance values were not available for comparison against model predictions, ANN predictions were compared against LR and expected system responses.

In order to conduct this extended simulation exercise, both the ANN and LR models were initialized to the measured/interpolated conductance value for only the first monthly prediction. Using their first predicted

conductance value as the initial value for the second prediction period, this self-initializing process is repeated for both ANN and LR over the 46-month validation period. Thus, the prediction made with each model for time period n was then used to reinitialize the model for prediction period $n + 1$.

The ANN accurately reproduced available measured/interpolated conductance values early in the prediction horizon (Figure 7). The ANN went on to produce three distinct peaks with increasing and decreasing limbs representing three consecutive years with obvious seasonal changes in pumping extraction. The first 2 years lack measured/interpolated conductance values to compare ANN predictions against. Based upon some analytical modeling (Magelky et al. 2004) and professional judgment, the ANN appears to provide excellent predictions early in the prediction horizon. Accuracy, however, appears to diminish near the highest peak in the data set, where the ANN prediction curve begins to inflect upward (increasing slope) and peaks above 4500 units. Because the ANN, as shown by the sensitivity analyses, is most influenced by initial conductance, it may be over-responding to these relatively high initial conductance values because there are fewer learning patterns at the extreme values. Despite the temporary overshoot, the ANN gradually corrects and converges back to the measured/interpolated values near the final 1985 peak.

Over most of the first part of year 1, LR closely follows the ANN predictions. However, it appears to significantly underestimate conductance values and approaches a minimum of 300 $\mu\text{S}/\text{cm}$. Unlike ANN, LR is not able to recover, and while capturing the general rising and falling trends of conductance, underestimates conductance levels over the final 1.5 years, with significant discrepancies existing during months with higher measured levels.

Table 5
The Mean Absolute Prediction Error of ANN and LR Both With and Without Climate Input Variables

Prediction Period (d)	ANN (with climate input variables)	ANN (without climate input variables)	LR (with climate input variables)	LR (without climate input variables)
30	61.8	133.8	148.5	195.0
60	67.6	134.7	168.9	237.6
90	25.4	72.7	99.7	343.2

Note: Units are in $\mu\text{S}/\text{cm}$.

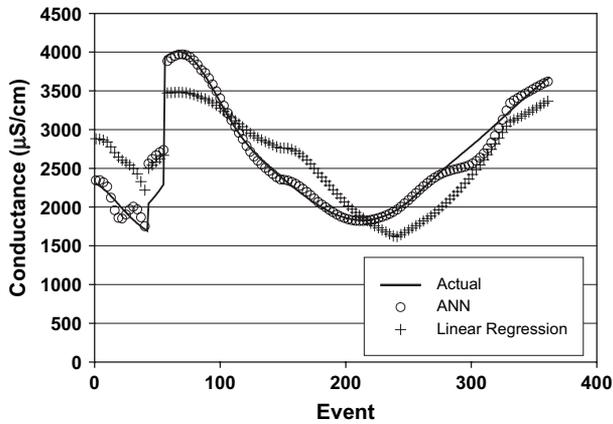


Figure 6. ANN and LR vs. measured/interpolated conductance values for the 90-d prediction period without climate variable inputs.

Conclusions

In this study, ANN technology was used to accurately predict highly dynamic conductance values due to vertical displacements in the brackish zone and salt water–fresh water interface in a fresh water lens aquifer in response to variable pumping and climate conditions. Prediction periods ranged from 30 d to several years, and the results were compared against both LR and measured/interpolated field data. The ANN approach provides a number of advantages over LR and other traditional physical-based modeling methods.

First, as nonlinear behavior becomes more pronounced, such as at the pumping well or under higher ground water extraction conditions, the ANN performance is not expected to decline significantly if at all because of its inherent nonlinear modeling capability (i.e., Kolmogorov’s theorem). Second, as the hydrogeology becomes more complex, with greater heterogeneity and/or less “ideal” environments (e.g., layered geology, fractured rock, limestone, etc.), the assumptions of simplified physical-based models become less appropriate, which is further exacerbated by model parameter uncertainty. Under these conditions, the ANN technology may provide superior real-time predictions with its nonlinear relationships between relatively easily measured variables.

However, physical-based models offer other advantages. For example, numerical advection-dispersion transport models can predict the movement of the brackish

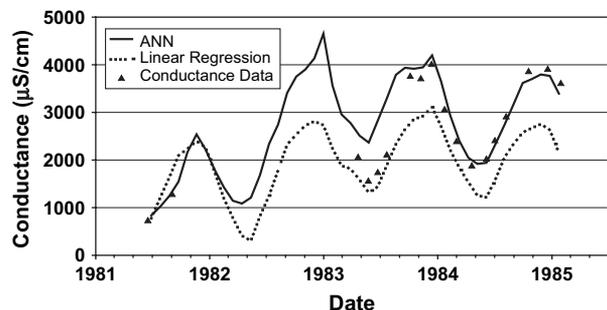


Figure 7. ANN vs. LR over the multiyear prediction period.

zone and interface, and resulting water quality conditions, at any location of interest within the modeled flow field. In addition, unlike an ANN, which cannot extrapolate to new system conditions, a physical-based model has the ability to predict changes many years into the future (e.g., decades or centuries) by accounting for projected changes in human activities and pumping stresses (e.g., new wells).

Another important benefit of the ANN technology as demonstrated in this study is that it can provide insights into important cause and effect relationships that foster an improved understanding of the physical system dynamics. An improved system understanding can help improve data collection strategies and future modeling efforts (both ANN and physical based). The fact that ANN models are “data driven” and can be reinitialized to real-time conditions (e.g., conductance level) makes the technology an ideal complement to continuous data stream systems (e.g., SCADA). This convergence of technologies is expected to increase predictive accuracy and thereby produce more effective real-time aquifer management strategies.

Effective ANN-based management would in many cases require installation of a network of monitoring wells at strategic locations for adequately assessing water quality conditions in the ground water system. Using these data, the ANN would be trained to predict water quality at specific “indicator” locations in the coastal aquifer associated with saline water movement induced by pumping and climate conditions. It is envisioned that with this type of system, the ANN technology in conjunction with an automatic data collection system can be used to balance short-term objectives (e.g., meeting monthly demand during peak season) with long-term consequences (e.g., salt water upcoming/intrusion or dewatering of critical habitat marshlands). Integration of real-time prediction capability into the management system can help the operator identify appropriate pumping extractions that meet expected demand requirements but do not pose an unacceptable risk to water quality conditions or the environment in the long term. As water demand increases in coastal areas and water supplies diminish, this type of forecasting and management tool may prove to be of great benefit in many areas around the world.

Acknowledgments

We gratefully acknowledge the comments provided by the three anonymous reviewers, which substantially improved this paper.

References

- Anderson, M., and W. Woessner. 1992. *Applied Groundwater Modeling*. San Diego, California: Academic Press Inc.
- ASCE Task Committee on Application of Artificial Neural Networks in Hydrology. 2000a. Artificial neural networks in hydrology. I: Preliminary concepts. *Hydrologic Engineering* 5, no. 2: 115–123.
- ASCE Task Committee on Application of Artificial Neural Networks in Hydrology. 2000b. Artificial neural networks in

- hydrology. II: Hydrologic applications. *Hydrologic Engineering* 5, no. 2: 124–137.
- Camp Dresser & McKee Inc. 1985. *Update of the Water Supply Plan for the Provincetown Water System*. Boston, MA: CDM.
- Cape Cod Planning and Economic Development Commission. 1989. *Truro/Provincetown Aquifer Assessment and Groundwater Protection Plan*. Barnstable, MA: CCPEDC.
- Coppola, E. 2000. Optimal pumping policy for a public supply wellfield using computational neural network with decision-making methodology. Ph.D. diss., Department of Hydrology and Water Resources, University of Arizona.
- Coppola, E., M. Poulton, E. Charles, J. Dustman, and F. Szidarovszky. 2003a. Application of artificial neural networks to complex groundwater management problems. *Natural Resources Research* 12, no. 4: 303–320.
- Coppola, E., F. Szidarovszky, M. Poulton, and E. Charles. 2003b. Artificial neural network approach for predicting transient water levels in a multilayered groundwater system under variable state, pumping, and climate conditions. *Hydrologic Engineering* 8, no. 6: 348–359.
- Coppola, E., A. Rana, M. Poulton, F. Szidarovszky, and V. Uhl. 2005. A neural network model for predicting water table elevations. *Ground Water* 43, no. 2: 231–241.
- Coulibaly, P., F. Ancil, R. Aravena, and B. Bobee. 2001. Artificial neural network modeling of water table depth fluctuations. *Water Resources Research* 37, no. 4: 885–896.
- Gelhar, L. 1993. *Stochastic Subsurface Hydrology*. Englewood Cliffs, New Jersey: Prentice Hall.
- Gumrah, F., B. Oz, B. Guler, and S. Evin. 2000. The application of artificial neural networks for the prediction of water quality of polluted aquifer. *Water, Air, and Soil Pollution* 119, no. 1: 275–294.
- Guswa, J.H., and D.R. LeBlanc. 1985. Digital models of ground-water flow in the Cape Cod aquifer system, Massachusetts. USGS Water-Supply Paper 2209. Boston, MA: USGS.
- Magelky, R.D., C.F. McLane, E. Coppola Jr., M. Poulton, and F. Szidarovszky. 2004. Analytical modeling of saltwater upconing for wellfield protection. Abstract Proceedings of the American Water Resources Association 2004 Annual Conference, Orlando, Florida. Middleburg, VA: AWRA.
- Masterson, J.P. 2004. Simulated interaction between freshwater and saltwater and effects of ground-water pumping and sea-level change, Lower Cape Cod Aquifer System, Massachusetts. USGS Scientific Investigations Report 2004-5014. Reston, VA: USGS.
- Oldale, R.N. 1969. Seismic investigations on Cape Cod, Martha's Vineyard, and Nantucket, Massachusetts. USGS Professional Paper 650-B. Reston, VA: USGS.
- Rao, S.V.N., B.S. Thandaveswara, S. Murty Bhallamudi, and V. Srinivasulu. 2003. Optimal groundwater management in deltaic regions using simulated annealing and neural networks. *Water Resources Management* 17, no. 6: 409–428.
- Rogers, L.L., and F.U. Dowla. 1994. Optimization of groundwater remediation using artificial neural networks with parallel solute transport modeling. *Water Resources Research* 30, no. 2: 457–482.
- Voss, C.I., and W.R. Souza. 1987. Variable density flow and solute transport simulation of regional aquifer containing a narrow freshwater-saltwater transition zone. *Water Resources Research* 23, no. 10: 1851–1866.
- Yakowitz, S., and F. Szidarovszky. 1989. *Introduction to Numerical Computations*, 2nd ed. New York: Macmillan Publishing Company.



5th International Conference on Pharmaceuticals and Endocrine Disrupting Chemicals in Water

March 13–15, 2006
Costa Mesa Hilton
Costa Mesa, California

Evidence suggests that environmental exposure to some anthropogenic chemicals may result in disruption of endocrine systems in human and wildlife populations. Concerns about endocrine disrupting chemicals appearing in the environment, water, soil, and foodstuffs have focused considerable national and international interest in their origin, transport, fate, and manner of detection. Research is pointing to a range of diseases in humans and wildlife that are associated with exposure to endocrine disrupting chemicals.

Cosponsors:

- U.S. EPA National Risk Management Research Laboratory
- U.S. Geological Survey Toxic Substances Hydrology Program
- Technical University of Berlin
- Orange County Groundwater Replenishment System
- Kompetenzzentrum Wasser Berlin

Visit www.ngwa.org for details concerning submissions and presentations or call 800 551.7379, ext. 546.