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Abstract: Determining the location of the contaminant source is important for improving remediation and site management decisions at many contaminated groundwater sites. At large sites, numerical flow and transport models have been developed that use historical measurement data for calibration. A well-calibrated model is useful for predicting plume migration and other management purposes; however, it is difficult to back out the source with these forward flow and transport models. We present a novel technique utilizing Artificial Neural Networks (ANNs) to backtrack source location and earlier plume concentrations from recent plume information. For proof-of-concept, two tracer tests (a non-point-source and a point-source) were performed in a large-scale (10’×14’×6’) groundwater physical model. The physics-based flow and transport model (MODFLOW 2000 and MT3DMS) was calibrated using the data from the non-point-source tracer test and validated using the point source tracer test data. ANNs (e.g. counterpropagation) were trained using the calibrated model predictions and compared to actual data. Results show this to be a promising method for determining earlier plume and source locations.

***Keywords**:* Artificial Neural Networks; Source identification; Groundwater modeling; Counterpropagation

1. INTRODUCTION

Identifying and delineating the source of a contaminant plume is important for improving subsurface remediation and site management decisions at many contaminated groundwater sites. Numerical flow and transport models are being extensively used to simulate and predict plume concentrations at sites that have sufficiently large amounts of data such that accurately calibrated simulation models can be utilized in the design process. These process-based simulation models provide valuable information for selecting and/or optimizing remediation strategies and long-term monitoring designs. Although a well-calibrated model is useful for predicting plume migration and other management purposes; it is difficult to solve the inverse problem and back out the source with these forward flow and transport models. The inverse problem is often ill-posed [*Skaggs and Kabala*, 1994] because it is extremely sensitive to errors in the measurement data, and might result in unstable numerical schemes when an existing transport model is run in reversed time [*Skaggs and Kabala*, 1994]. As a result, a number of methods have been developed for these inverse problems, such as nonlinear optimization modeling [e.g. *Aral, et al.*, 2001], geostatistical inverse modeling [e.g. *Michalak and Kitanidis*, 2004], and chemical profiling [e.g. *Morrison*, 2000, 2000, 2000]. *Bagtzoglou* [2003] presented a Reversible-Time Particle Tracking Method (RTPTM), but it is only applicable for one-dimensional problems.

We present a technique that combines Artificial Neural Networks (ANNs) with a flow and transport model to backtrack the source location and earlier plume concentrations from recent plume information. For proof-of-concept, two tracer tests (a non-point-source and a point-source) were performed in a large-scale (10’×14’×6’) groundwater physical tank. This method takes full advantage of the available physics-based flow and transport model that has been calibrated for these tank experiments. Once trained, the ANN is capable of mapping the model results in a more computationally efficient manner, saving time for optimizing remediation strategies or long-term monitoring designs that require repeated modeling effort. The trained ANN can also simulate the plumes in reverse to find a reasonable estimate of the contaminant source, endowing the flow and transport model with backtracking capability.

2. BACKGROUND

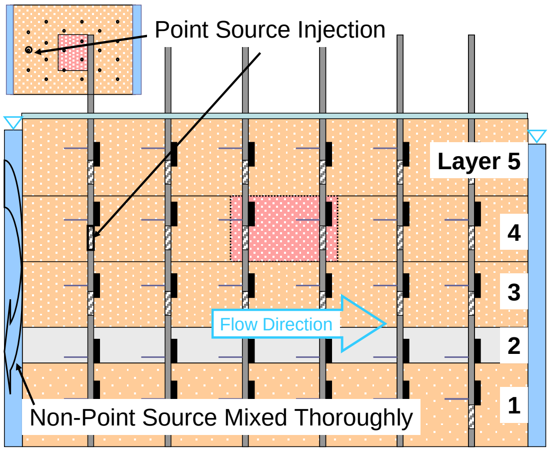
Increased efforts have been made to clean and protect groundwater resources. Groundwater numerical flow and transport models that are based on the physics of groundwater migration are well accepted as valuable tools for predicting contaminant plumes. These models are used in two different ways. (1) Models are run forward to delineate and forecast the future of contaminant plumes. This method plays a critical role in designing remediation strategies and long-term monitoring optimization. Although the costs associated with long-term monitoring may be large, it is required for contaminated sites or sites prone to be contaminated (*e.g.* lined or unlined landfills) by the US EPA. Models are used to identify areas at risk of being contaminated, direct monitoring schemes and improve remediation strategies. (2) Models may be run backward to delineate earlier contaminant plumes and identify the location of contaminant sources. This forensic approach is often important for distributing costs among responsible parties for remediation.

3. METHODS

Two tracer tests were performed in a large-scale (10'x14'x6') physical model of a sand and silt layered aquifer. The physical model has a precisely defined stratigraphy. It comprises five layers (from bottom to top): a coarse sand layer, a silt layer, a medium sand layer, a medium sand layer with a fine sand rectangular block in the middle, and a medium sand layer (see Figure 1a). Constant head inlet and outlet reservoirs were constructed to feed into/from the in-tank reservoirs, thus creating a fixed water gradient across the tank. The tank has a dense sampling system, and a sophisticated data acquisition and control system to collect sufficient data in real time for various experimental applications (Figure 1b). There are 21 PVC pipes within the tank; each contains probes and sensors at five depths (for a total of 105 locations), and each is screened for pumping groundwater at four depths (84 locations). Probes and sensors include pressure transducers, Time Domain Reflectometry (TDR) probes, thermocouples and point sampling probes.

3.1 Non-Point Source Tracer Test

Ammonia chloride was chosen as the tracer for both the non-point and point source tracer tests. The advantages compared to other tracer salts are three-fold: (1) the change in density as compared to pure water is low; (2) it is generally nonreactive with the media; and (3) it has high electrical conductivity that makes it easy to detect with the TDR probes. For the non-point test, a concentrated salt solution was mixed thoroughly in the in-take inlet reservoir to ensure a constant concentration (1000 mg/L) and a plug flow tracer test. A constant head difference of 4.6 cm between the inlet and outlet reservoir was maintained, and influent solutions (also 1000 mg/L ammonia chloride) were continued for five days. After five days, the feed solution was changed to tap water. The 105 TDR probes were used to determine electrical conductivity which was then converted to concentrations. Measurements were collected at approximately 20-minute intervals at various TDR probe locations for 9 days.



(a)

(b)

Figure 1. (a) Tank representation showing well/probe locations and fine sand lens; (b) Tank plan view and cross-sectional view.

3.2 Point Source Tracer Test

Sixty-three TDR probes positioned in the top three layers were used to determine the electrical conductivity which was converted into concentration data using the method of *Wraith, et al.* [1993]. The ammonia chloride solution (1000 mg/L) was injected at 1.5 L/hr constant flow rate into one of the screened intervals within the medium sand layer with fine sand lens (fourth layer from bottom, see Figure 1a). Measurements were collected at approximately 15 minute intervals for 19 days.

3.3 Flow/Transport Modeling

A number of models have been developed for flow/transport modeling, for example MODFLOW [*Harbaugh, et al.*, 2000], MT3D [*Zheng and Wang*, 1999], RT3D [*Clement, et al.*, 1998] and MINTRAN. *Gorelick* [1983] and *Mangold and Tsang* [1991] present an excellent review of groundwater modeling. *Oreskes, et al.* [1994] report the methods for model verification, validation and confirmation.

A combination of MODFLOW 2000 and MT3DMS was used in this paper. MODFLOW is a three-dimensional finite-difference computational model that numerically solves the ground-water flow equation for a porous medium [*Harbaugh, et al.*, 2000]. The modular 3-Dimensional Transport model MT3DMS has a comprehensive set of capabilities for simulating the advection, dispersion/diffusion, and chemical reactions of contaminants in groundwater flow systems under general hydrogeologic conditions [*Zheng and Wang*, 1999].

The numerical flow and transport model was calibrated using the data from the non-point-source tracer test. There were nine layers in the numerical model, with an approximately square grid spacing (70 by 100 elements) for each layer. Model calibration was conducted using hydraulic conductivity, porosity and dispersion values calculated from extensive analysis of the breakthrough curves generated from the non-point source tracer test, and then making slight modifications (consistent with experimental error) to visually achieve the best fit. Concentration data at thirty-six observation points collected from nine PVC wells (four in each) were used for comparison with model simulations. The model approximated the data very well. The calibrated flow and transport model was then validated using the point-source tracer test data. Model predictions showed similar plumes to the experimental data.

3.4 Counterpropagation ANNs Training and Interpolation

An Artificial Neural Network (ANN) is an information-processing paradigm inspired by the way biological nervous systems process information. In general, a supervised ANN consists of two phases, a *training* phase and an *operational* phase. During training, a set of inputs and associated known outputs are fed into the ANN. The internal weights are iteratively adjusted until the mapping between inputs and outputs meet some specified convergence criterion. The weights are then fixed and used to interpolate data points not used in previous ANN training. *Maier and Dandy* [1996] presented a method using ANN to forecast salinity, and *Zhang and Stanley* [1997] used a ANN modeling scheme to predict raw-water color. An excellent review about forecasting water resources variables using ANN was presented by *Maier and Dandy* [2000]. *Govindaraju* [2000] provided a good review of the application of ANNs in environmental engineering. *Rogers and Dowla* 1994 used a feed-forward backpropagation ANN as a surrogate for the flow and transport simulator used to perform groundwater remediation optimization at the Lawrence Livermore National Laboratory in Livermore, California.

A feed-forward counterpropagation ANN was used in this paper and is depicted in Figure 2. *Hecht-Nielsen* [1987, 1988] proposed counterpropagation as a method to combine an unsupervised Kohonen ANN with a supervised Grossberg ANN. This combination synthesizes complex classification problems and attempts to minimize the number of processing elements and training time.

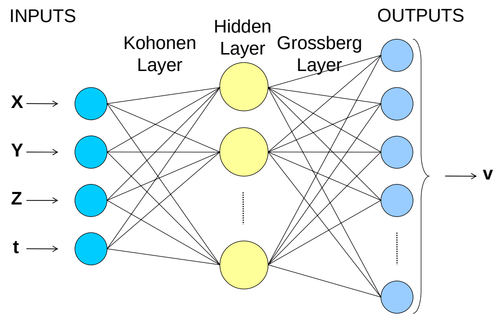


Figure 2. Schematic of the feed-forward conterpropagation ANN comprised of an input vector corresponding to the time and spatial location of known classified concentration values.

Simulated model concentration data, which is normalized by dividing by C_0, from time periods t = 1, 3, 5, 7, 9, 11, 13, 15, 17 and 20 days were used to train the counterpropagation ANN. For the purpose of determining the location of the contaminant source, no concentration was assumed at day t = -1, which is reasonable because it is known that no ammonia chloride was introduced into the tank until day t = 0. Before training, the output normalized concentration values (v), originally ranging from 0 to 1, were classified into 21 classes as indicated in Table 1. The input data comprise the time and x, y, z coordinate location of measured concentration values for all training time periods. The corresponding classified concentration value at that specified location and time is used as the output data. During the training process, the weights are adjusted so that the output maps the classified target concentration to a predefined root-mean-square error value (10^{-6} in this study).

After convergence, the weights are fixed. The interpolation phase, modified with an inverse distance method, uses the fixed weights for prediction. The three closest patterns stored in the hidden layer (two points backward in time and one point forward in time) are selected and a weighted average is calculated as the predictor. For example, to estimate the plume at t = 6, the data at t = 3, 5, and 7 will be used.

Table 1. Classification of the concentration value into 21 classes with intervals=0.05 units

Class	Concentration (v)
1	0
2	$0<v\leq 0.05$
3	$0.05<v\leq 0.1$
⋮	⋮
n*	$0.05\times(n-2)<v\leq 0.05\times(n-1)$
⋮	⋮
21	$0.95<v\leq 1$

*n=2, 3, 4…, 21

4. RESULTS AND DISCUSSION

The concentration plumes (isocontours ≥ 0.5) estimated using the modified counterpropagation network were compared to the model simulation results. Select comparisons for time = 3, 8 and 17 days are shown in Figure 3. Results indicate that the counterpropagation ANN performs well for predicting the plume patterns (Figure 3). Forecasts of the ANN 0.5 isocontour on the 19th day (the end of the tracer test) were compared to the flow and transport model prediction. In addition, the 0.5 isocontour was backed out using the ANN at t = 0 days (the beginning of the contaminant release). The prediction of the source (see Figure 4a) was close to the injection spot, indicating that this is a promising method for backtracking the earlier plume and identifying the location of the contaminant source.

This method takes advantage of the available physics-based models that may already have been developed for contaminated sites, while avoiding many of the complications associated with solving the inverse problem. Once trained, the ANN is capable of simulating the model results in a more computationally efficient manner. This may save large amounts of computational effort especially when applied to optimization remediation problems and/or long-term monitoring design efforts that require repeated (often hundreds or thousands) process-based simulations. Our ANN method enables the system to be updated in real-time by combining physics-based model predictions and sparsely collected site data. It should be noted; however, that the traditional forward-feedback counterpropagation ANN used in this research acts as an interpolation method and/or pattern-lookup system; and perhaps is not the best ANN for forecasting or extrapolating estimates of concentration at times outside of the training data set or for simulating the physics-based model. The counterpropagation ANNs are good at classification analysis, which can be viewed as a nearest neighbor (or nearest-means) classification method; while its forecasting capability is limited. The algorithm was modified to incorporate an interpolation procedure that averages the closest three training patterns using an inverse distance method to overcome such disadvantages.

5. CONCLUSIONS AND FUTURE RESEARCH

Artificial neural networks are useful computational tools for water quality modeling and this paper shows its usefulness for application to groundwater flow and transport problems. Once trained, ANNs are capable of approximating results quickly, which is important for real-time modeling and long-time monitoring optimization design. The ANNs can also back out the earlier plumes to better identify the contaminant source. Further research using other ANNs to improve performance and extend their application is still needed. A recurrent ANN [*Connor, et al.*, 1994] or a time series ANN [*Clouse, et al.*, 1997] will be used in the future to improve the prediction capability.

6. ACKNOWLEDGMENT

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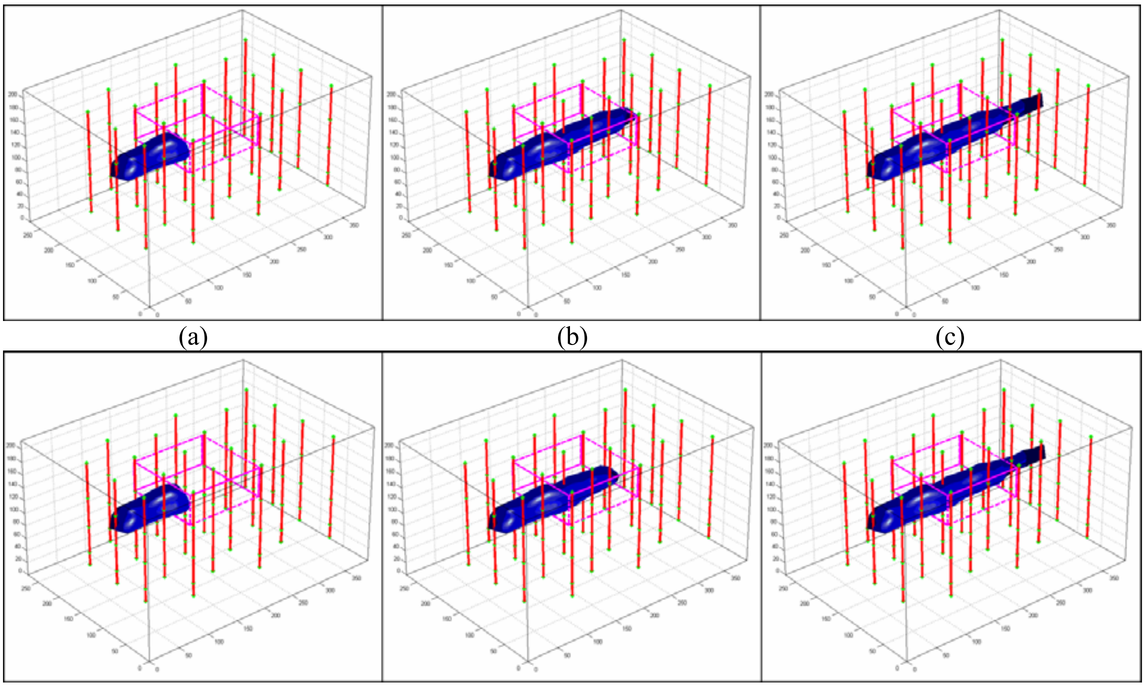
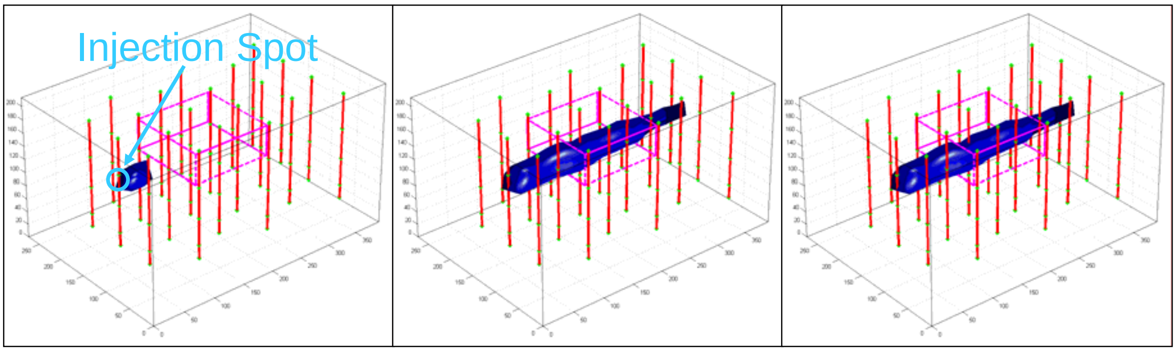


(a) (b) (c) (d) (e) (f)

Figure 3. 3-D flow/transport model estimates of NH_4Cl (a) time=3 days, (b) time=8 days and (c) time=17 days; and 3-D ANN estimates of NH4Cl at (d) time=3 days, (e) time=8 days and (f) time=17 days. The iso-contour indicates where normalized concentrations exceed 0.5.



(a) (b) (c)

Figure 4. 3-D ANN estimates of NH_4Cl at (a) time=0 days and (b) time=19 days; and (c) flow/transport model prediction at time=19 days. The iso-contour indicates where normalized concentrations exceed 0.5.

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