7 ARTIFICIAL NEURAL NETWORKS AND THEIR APPLICATIONS

Introduction

Artificial Neural Networks are composed of many simple elements called neurons connected with each other through links. The neuron model as shown in Figure 7-1 shows how a network transforms its input into and output.

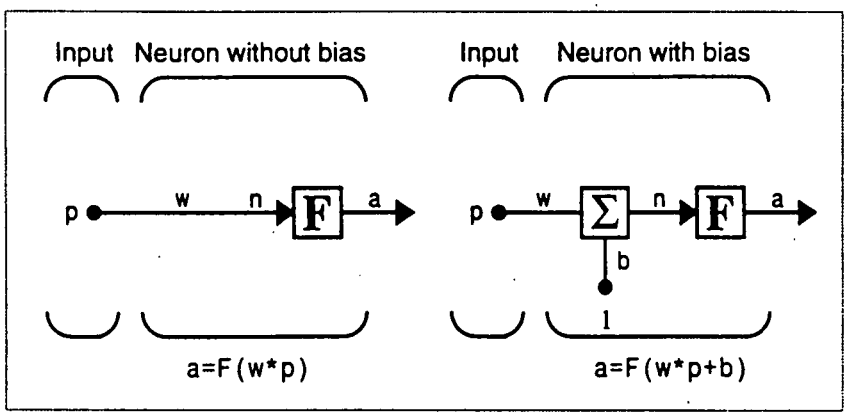

Figure 7-1. Single Input Neuron (Matlab 1994)

A neuron with a single input and output is shown in Figure 7-1. The input **p** is multiplied by a weight **w**. A bias term is then added to the weighted input. The transfer function **F** takes this sum and produces output **a**. **w** and **b** are adjustable scaler parameters of the neuron. The transfer function is defined by a function, such as log–sigmoid. A few of the common transfer functions are illustrated in Figure 7-2.

An extension of the single input–single output neuron is the multiple input-single output neuron as shown in Figure 7-3. Two or more such neurons may be combined to form a layer of neurons as shown in Figure 7-4. Two or more such layers in series as shown in Figure 7-5 constitute an artificial neural network.

Figure 7-5 illustrates a feed–forward type of ANN. If the outputs are fed back as inputs the ANN is a recurrent type.

Why Use ANNs

Artificial Neural Networks are widely used and well–suited for multiple non-linear regression. They can be interpreted as predicting the expected value of the conditional target distribution as a function of the input pattern. Neural networks are universal approximators, that is they are capable of modeling any function with a finite number of discontinuities to any desired degree of accuracy given sufficient number of hidden neurons. Thus no prior assumptions, such as determination of transfer functions, need to be made about the nature of the relationship between the inputs and outputs. Minimal pre–processing is required and different types of inputs can be used in the same network. Once calibrated ANNs are fast and reasonably accurate.

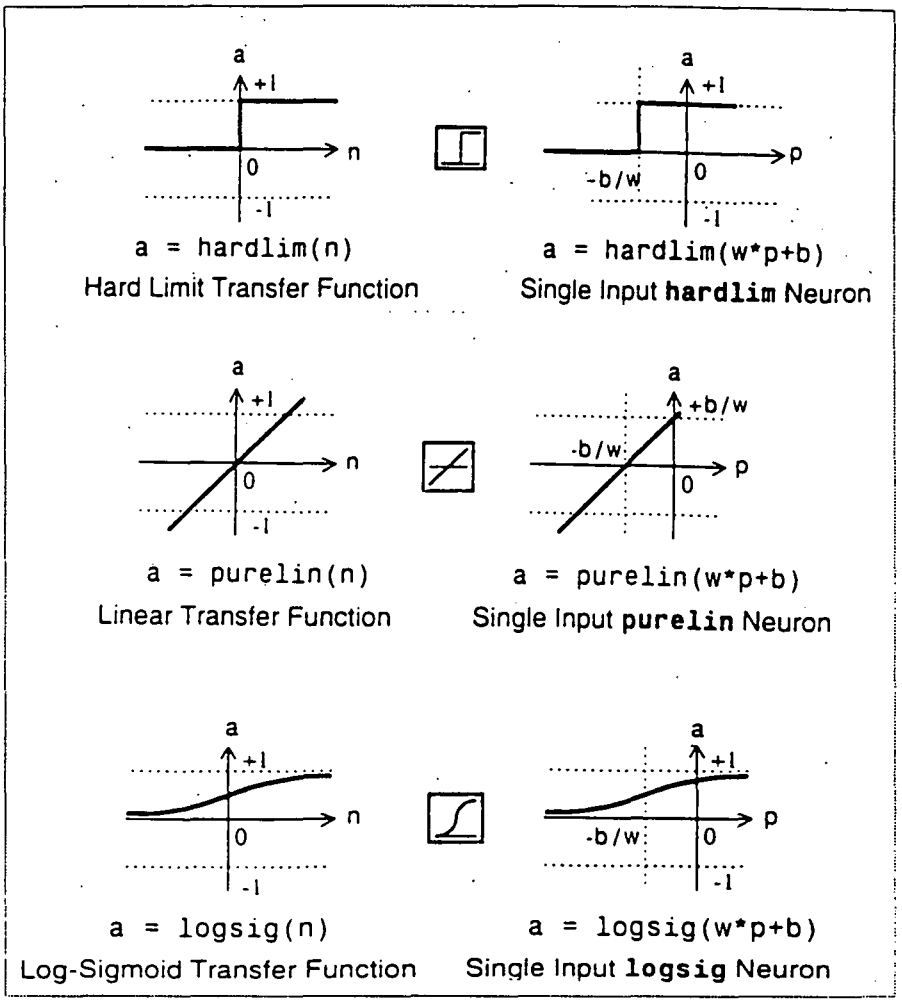

Figure 7-2. Transfer Functions (Matlab 1994)

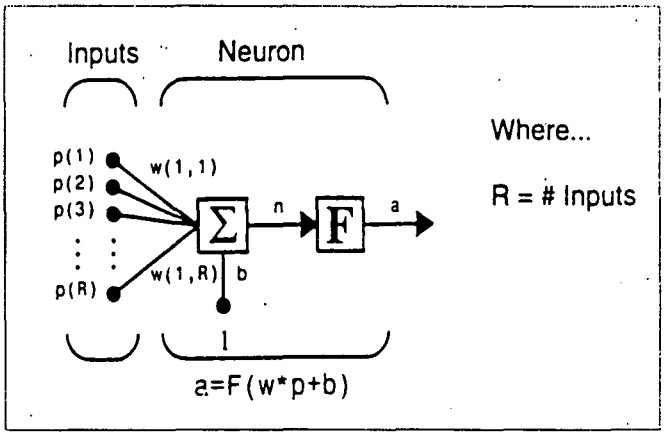

Figure 7-3. Multiple Input Neuron (Matlab 1994)

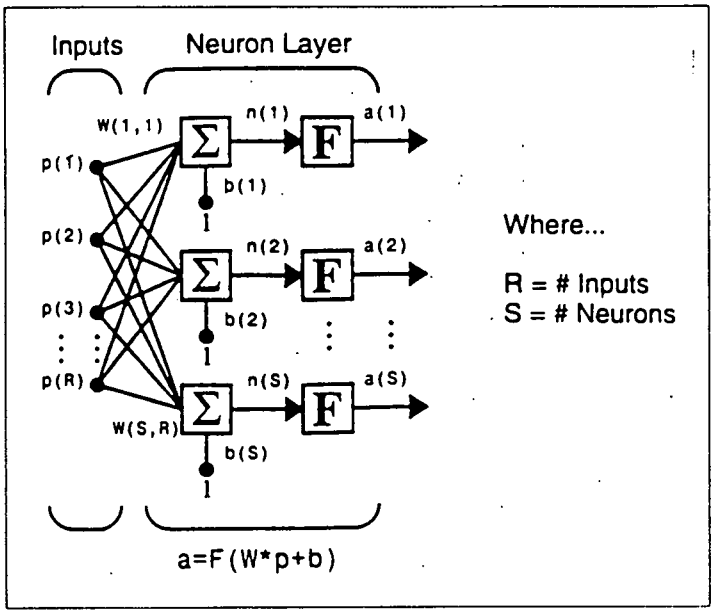

Figure 7-4. Single Layer of Neurons (Matlab 1994)

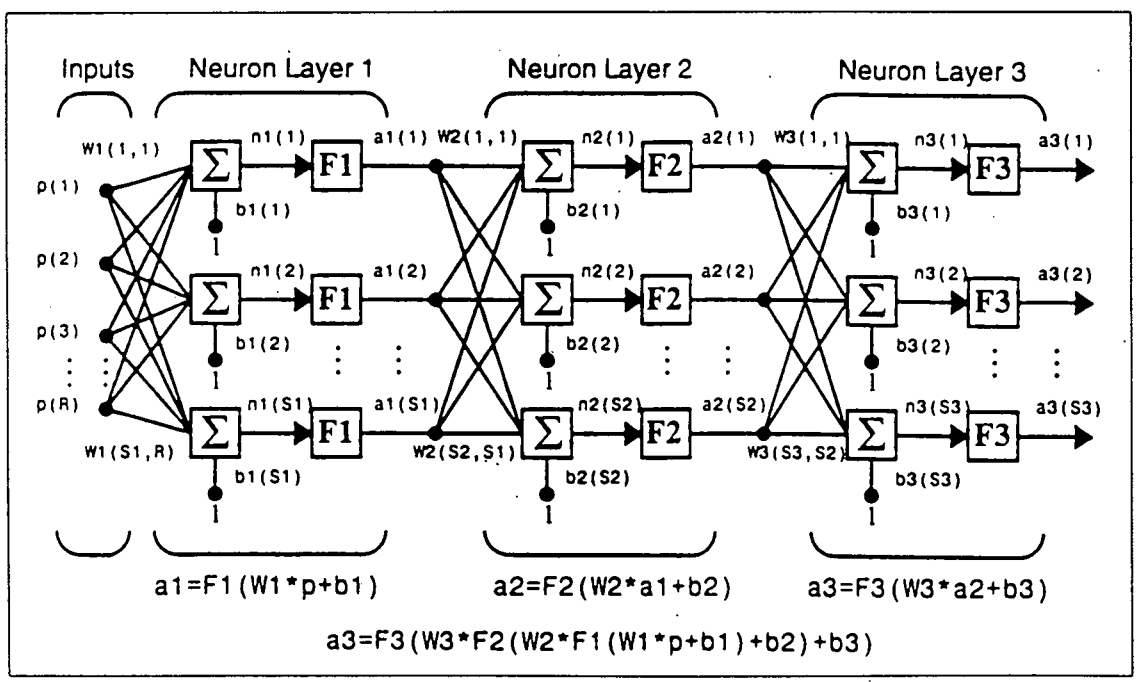

Figure 7-5. Neural Network (Matlab 1994)

Applications at DWR

Presently, the Department of Water Resources has applied ANNs in the following areas:

- Estimation of salinity from flows and gate positions in the Sacramento-San Joaquin Delta. (See Chapter 9.)
- Estimation of THM species. (See Chapter 8.)

Future applications proposed are:

- A real time salinity prediction model for a day to day basis.
- Conversion equations for conversion between different measuring techniques of salinity such as TDS, EC, and ion concentrations.
- Fish take estimation from flow conditions in the Sacramento-San Joaquin Delta.
- Reasonable emulation of sophisticated models, such as ground water models, to have significant cuts in run-time while giving reasonable results.

Almost anywhere regression is used, results could be more accurate by using the ANNs.

References

Neural Network Toolbox User's Guide. Jan. 1994. Math Works, Inc.

8 DISINFECTION BY-PRODUCT FORMATION

Work continued by Delta Modeling staff to develop, calibrate and validate a model of trihalomethane (THM) formation potential in Delta waters. This year emphasis was placed on refining the Delta Island Consumptive Use (DICU) model, a key model in simulating mass loading of organic THM precursors in the Delta. (Refer to Chapter 5 for details on this work.)

Work was also conducted this year to improve on the THM predictive formulation discussed in last year's annual report (Methodology 1994). Calibration and validation of the improved formulation were conducted with the same data sets reported in last year's annual report. The formulation proposed last year included three components: a log-linear total THM or TTHM predictive equation developed by Malcolm Pirnie Inc. in support of EPA's Water Treatment Plant Simulation Program (Bay-Delta 1993); the bromine distribution factor relationships developed by Hutton and Chung (1994); and a bromine incorporation factor function calibrated with the data set reported in last year's annual report. The TTHM and bromine incorporation factor component were improved this year through the use of an artificial neural network (ANN).

ANN Structure

The Stuttgart Neural Network Simulator (SNNS), a public domain computer code, was trained to predict values of TTHM (in µg/L) and bromine incorporation factor. The ANN was given input values for bromide concentration, the product of dissolved organic carbon (DOC) concentration and ultraviolet absorbance at 254 nm (UV-254), available chlorine dose defined as chlorine dose minus 7.6 times ammonia concentration as nitrogen, reaction time, temperature, and pH. A feed-forward ANN, with five neurons in the first hidden layer and three neurons in the second hidden layer, was trained to minimize the percentage difference between observed and predicted values. A log sigmoid function was specified as the activation or transfer function. Prior to training, input calibration data were log transformed. Output calibration data were not log transformed. However, values of TTHM were scaled between 0.2 and 0.8 and values of bromine incorporation factor were scaled between 0.01 and 0.8.

Model Calibration and Sensitivity

A comparison of predicted and observed TTHMs and bromine incorporation factors for the calibration data set is shown in Figures 8-1 and 8-2, respectively. The trained networks generally provide a good fit to the observed data. Although Figure 8-1 reveals outliers when TTHM formation exceeds 250 µg/L, such conditions are well beyond those that will normally be observed when water utilities operate to meet the current 100 µg/L drinking water standard.

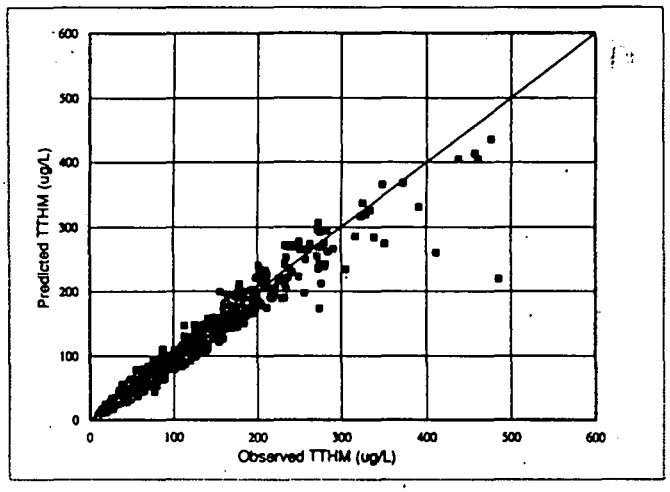

Figure 8-1. TTHM ANN: Calibration Results

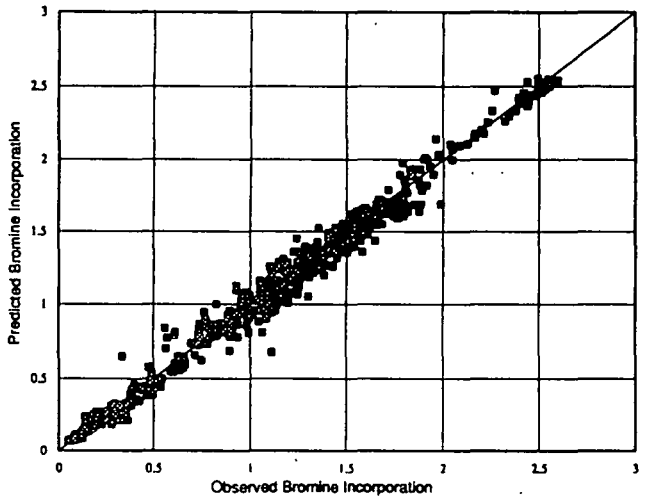

Figure 8-2. Bromine Incorporation Factor ANN: Calibration Results

The trained feed-forward networks were tested for sensitivity under "low" and "high" bromide levels, defined as 0.1 mg/L and 0.5 mg/L, and the following base conditions: DOC = 3 mg/L, UV-254 = 0.09 cm^{-1}, chlorine dose = 3 mg/L, NH_3-N = 0 mg/L, reaction time = 3 hours, temperature = 25°C, and pH = 8.2. The trained TTHM network demonstrates sensitivities to input variables that are similar to the log-linear TTHM predictive equation with one exception. While the log-linear formulation is insensitive to changes in DOC concentration and highly sensitive to changes in UV-254, the neural network formulation (which considers the product of DOC and UV-254 to be one input) is sensitive to both DOC and UV-254. These values were consolidated into one neural network input as they are strongly correlated.

The trained bromine incorporation factor network predicts decreasing values with increasing DOC, UV-254 and chlorine dose at both bromide levels and increasing values with increasing bromide and ammonia concentrations. The network was fairly insensitive to changes in reaction time, temperature, and pH. Therefore, these input variables were manually pruned prior to final training of the network.

Model Validation

The new formulation gives superior validation results to the one proposed last year. Figures 8-3(a) through 8-3(d) show the relative frequency of percent deviations between predicted and observed THM species concentrations for both formulations. The new formulation gives predictions within ± 30 percent of observed values 72 percent of the time for chloroform, 83 percent of the time for dichlorobromomethane, 88 percent of the time for chlorodibromomethane, and 93 percent of the time for bromoform. Figure 8-4 shows a similar comparison between predicted and observed TTHM values. The new formulation gives TTHM predictions within ± 30 percent of observed values 92 percent of the time and gives predictions within ± 10 percent of observed values 64 percent of the time. Percent deviations were computed only when observed concentrations were greater than or equal to 5 µg/L. Further efforts are planned to optimize neural

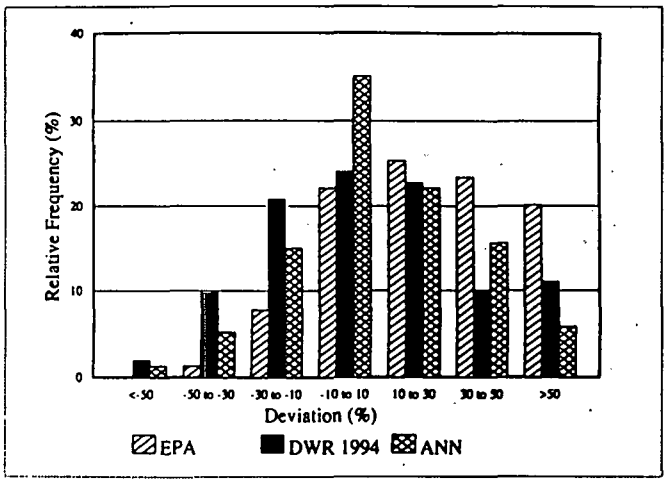

Figure 8-3a. Deviation Between Predicted and Observed Chloroform Concentrations: Validation Results

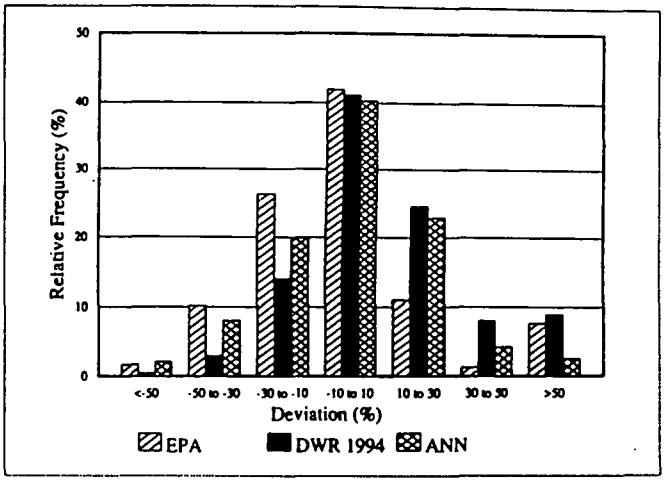

Figure 8-3b. Deviation Between Predicted and Observed Dichlorobromomethane Concentrations: Validation Results

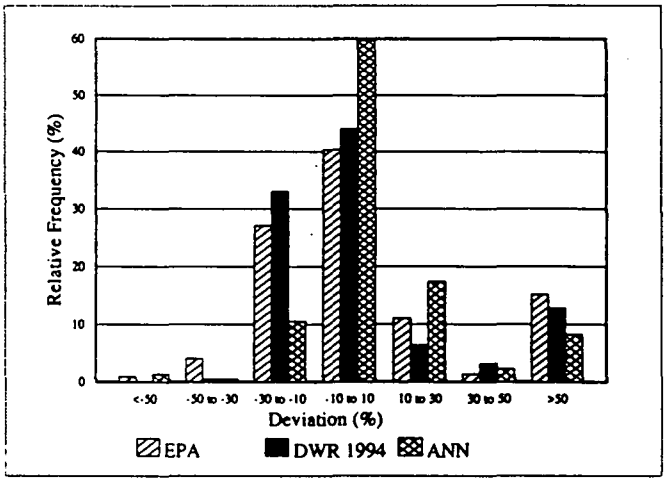

Figure 8-3c. Deviation Between Predicted and Observed Chlorodibromomethane Concentrations: Validation Results

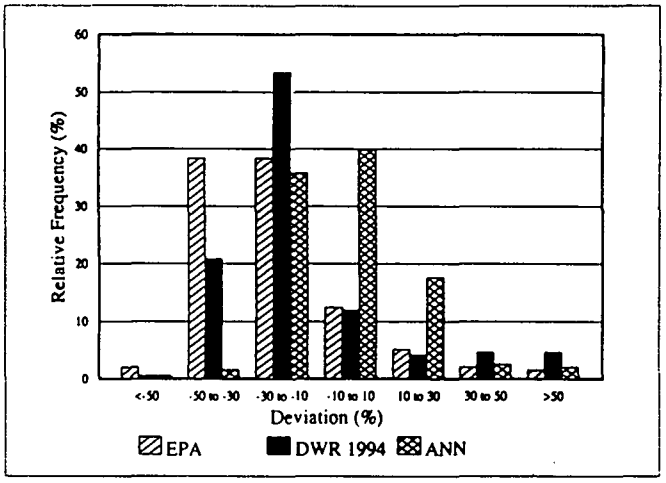

Figure 8-3d. Deviation Between Predicted and Observed Bromoform Concentrations: Validation Results

network performance in predicting TTHM and bromine incorporation factor.

Deviations associated with EPA's log-linear THM equations are also presented in Figures 8-3(a) through 8-3(d) and 8-4 for comparison. By correcting predicted values to be consistent with EPA's total THM equation (USEPA 1992), performance was enhanced over that reported in last year's annual report. However, these equations still provide inferior validation results. The EPA formulation gives predictions within ± 30 percent of observed values 55 to 56 percent of the time for chloroform and bromoform and 78 to 79 percent of the time for the remaining species. The EPA formulation gives TTHM predictions within ± 30 percent of observed values 90 percent of the time and gives predictions within ± 10 percent of observed values 48 percent of the time.

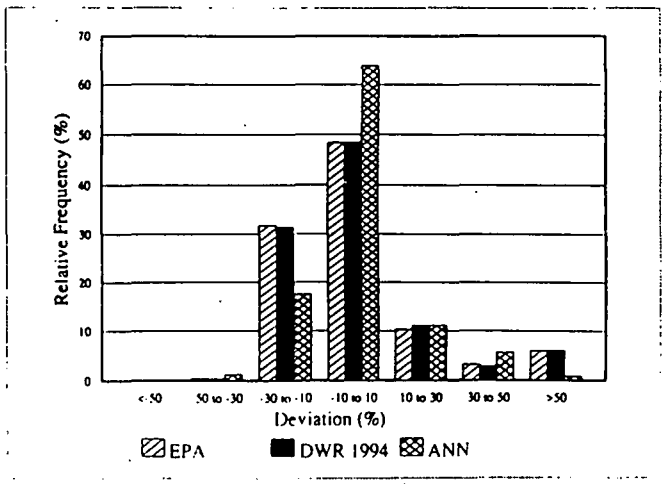

Figure 8-4. Deviation Between Predicted and Observed Total THM Concentrations: Validation Results

Bromine Distribution Factors

The bromine distribution relationships developed by Hutton and Chung (1994) were not recalibrated for the model validation effort because they provide good fits to both calibration and validation data sets. See Figures 8-5(a) through 8-5(d). Staff is also investigating the use of an alternate formulation discussed in last year's annual report. An optimization technique known as "adaptive simulated annealing" is being employed to calibrate model constants for the alternate formulation. As demonstrated in last year's annual report, this alternate formulation is a first step in modeling the formation of other disinfection by-products.

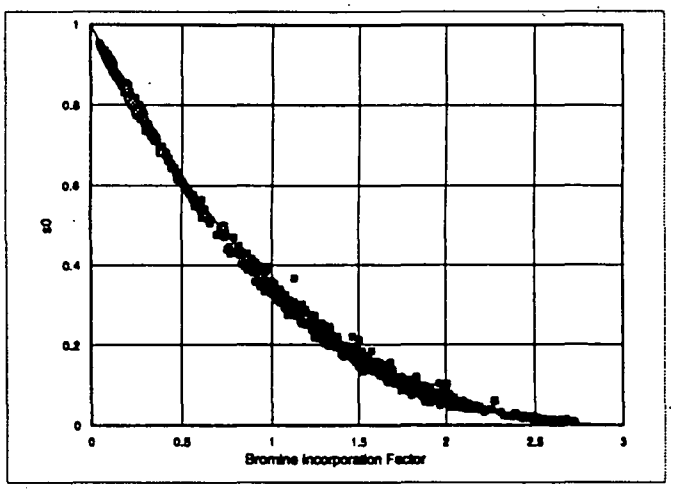

Figure 8-5a. Predicted and Observed S_0 as a Function of Bromine Incorporation Factor: Calibration and Validation Data

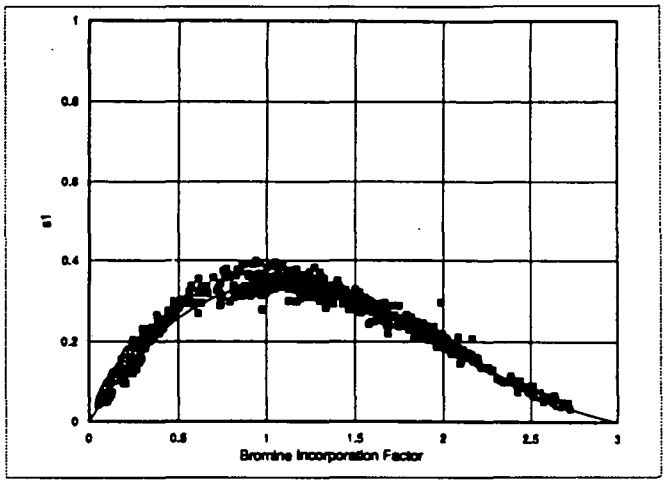

Figure 8-5b. Predicted and Observed S_1 as a Function of Bromine Incorporation Factor: Calibration and Validation Data

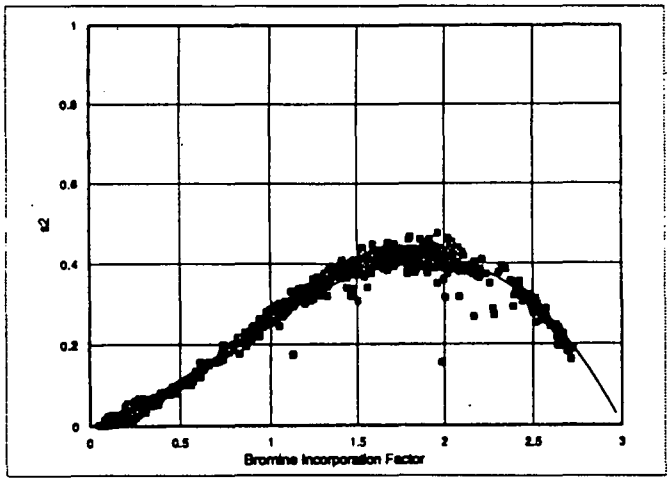

Figure 8-5c. Predicted and Observed S_2 as a Function of Bromine Incorporation Factor: Calibration and Validation Data

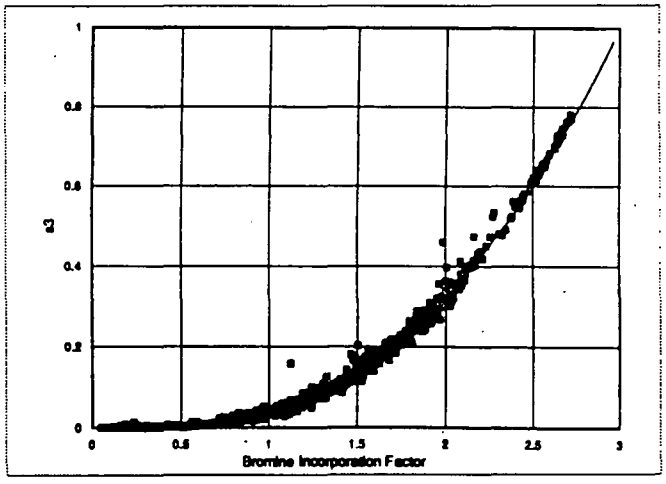

Figure 8-5d. Predicted and Observed S_3 as a Function of Bromine Incorporation Factor: Calibration and Validation Data

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Hutton, P. H. and Chung, F. I. (1994). "Bromine Distribution Factors in THM Formation." *J. Water Resources Planning. and Management*, ASCE, 120(1), 1-16.

"Methodology for Flow and Salinity Estimates in the Sacramento-San Joaquin Delta and San Francisco Bay" (1994). *Fifteenth Annual Progress Report to California State Water Resources Control Board*, California Dept. of Water Resources, Sacramento, CA, 5.1-5.13.

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9 CARRIAGE WATER

Definition of Carriage Water

Carriage water is defined as marginal export costs, that is, the extra water needed to carry a unit of water across the Delta to the pumping plants while maintaining a constant salinity. Or more practically, when the exports are increased by one unit, the Sacramento River flow is increased by one unit plus carriage water to maintain a constant Delta salinity.

Previous Work

It has been known for several years that the current method of estimating carriage water in DWRSIM, called the Minimum Delta Outflow routine, is not particularly accurate in individual years and a better method is needed. The Delta is a complex system and past attempts at developing a useful method for measuring carriage water and ultimately an MDO replacement always had at least one major flaw.

An attempt was made to search for carriage water directly in the historical data, that is, to find a period of time when Net Delta Outflow was fairly constant, but Sacramento River flow and exports were increasing. If carriage water existed, salinity at interior Delta stations should have increased. While there are a few times when this seems to be true (for example, summer 1979 and 1994), the salinity increase could also be explained by antecedent conditions, that is, previous to the period of constant NDO, NDO was much higher, and the salinity increase could be simply due to the Delta gradually reaching a new equilibrium. Thus it became apparent that only a model of the Delta could say anything about carriage water.

Most efforts at modeling the Delta and improving MDO involved using NDO, with perhaps some lagged NDO as memory, as the only input. However an NDO-only model cannot say anything about carriage water as it is defined above, nor can it deal with other questions about rim flow combinations, gate operations, and so on. Thus, a model is needed that can handle multiple inputs and nonlinear behavior. DSM has been used to investigate carriage water and related issues. Like all numerical models, it is rather slow compared to the time step needed for DWRSIM and therefore not a serious candidate for an MDO replacement. Even with a reduced channel grid, run times would be far longer than the current MDO routine. A "Transal" model was proposed as a fast and reasonably accurate method of modeling the Delta. In this method, flows and salt are tracked from and to different locations in the Delta. However, this type of model cannot be used directly with historical data and was therefore unacceptable.

Statistically–based models have been tried and found lacking; traditional time–series analysis is often linear or requires transformation to a stationary time–series, which renders the resulting model unsuitable as an MDO replacement.

Application of Artificial Neural Networks (ANNs)

Feed–forward ANNs are used to relate the flows to the salinity at interior and boundary locations in the Delta. Inputs to the model are the flow conditions and gate positions at various locations in the Delta, and the output is the salinity in the form of electrical conductivity. The ANNs provide a fast and reasonably accurate method of modeling the relationship between flows and water quality.

Salinity data, in the form of electrical conductivity, is used from Collinsville, Contra Costa Canal Pumping Plant 1, Clifton Court Forebay, Union Island and Jersey Point. Years 1981–1991 are used to calibrate the ANN model and years 1971–1981 are used to validate the ANN model. The years 1981–1991 were years in which salinity remained high for longer periods of time due to extended droughts, and to extract this information, the ANNs were trained on this set. The sum squared error criteria was used in evaluating the fit in calibration and validation data sets.

Approaches Tried and Experiments Done

MATLAB, Timothy Master's code and SNNSv3.3 were a few of the packages tried for training of the neural networks. SNNSv3.3 was chosen as it was a public–domain package and had the greatest variety of architectures available. Also, it undergoes major improvements every six months which keeps it updated. Radial basis, Feed–forward, Elman, Jordan, Cascade correlation, Time–delay and fully Recurrent were some of the neural network architectures that were tried. Radial–basis and Cascade correlation did well in calibration but did not do well on the validation set. Feed–forward, Elman, Jordan and Time–delay networks did equally well in calibration. Time–delay outperformed the Feed–forward, Elman, and Jordan networks slightly in the validation error. The best performance was that of the recurrent networks. At present Feed–forward networks are being used as it is the only network architecture for which SNNSv3.3 can output stand-alone C code. Also the Feed–forward networks give reasonable results with faster run–time. Preprocessing of inputs by taking logarithms and inverses was done to try to improve performance. No improvement in performance was noted in the calibration set while the error increased on the validation set. The number of hidden neurons and number of hidden layers required was experimented with to determine a network with enough flexibility to do well on the calibration set and yet generalize well enough to do well on the validation set. Pruning or link elimination of ANNs was done to improve its generalization characteristics. Memory of inputs play an important role in the prediction of salinity. Various memory lengths were experimented with to arrive at a reasonable memory length. Using individual components of Net Delta Outflow (NDO) such as boundary inflows and outflows, channel depletions, precipitation, and gate positions instead of a single lumped input NDO value lead to improved prediction of salinity. Daily, weekly, and monthly time steps were tried. An attempt to model seasonality was made by limiting data to summer time only and also by splitting the data set into quarters corresponding to the four seasons. No improvement was noted in the generalization properties of the network. Further studies will have to be done to incorporate the seasonality factor in the prediction.

Final ANN Structure

SNNSv3.3 was the public domain package used for the training and simulation of the networks. Feed–forward structure was chosen due to its faster run time and superior generalization characteristics. It was chosen over the recurrent networks due to the

unavailability of stand-alone C code generation for the recurrent type networks. No pre–processing of data was deemed necessary except for scaling the inputs and outputs to the range of 0.2 to 0.8. This was done so that the output would lie in the linear region of the log–sigmoid transfer function in the output layer. Two layers with four neurons in the first layer and two in the second layer were used for most locations. Memory of at least eleven weeks was needed in most locations and in some locations more memory was required. The daily time–step model was chosen as the December Water Quality Control Plan is written in terms of daily standards and for eventual use with a stage model. The individual components of flow were Channel Depletions (CD), Precipitation (PREC),Contra Costa Canal flow (CCC), East stream flows (EAST), San Joaquin River flow (SJR), Sacramento River flow (SAC), State Water Project Pumping (SWP), and Central Valley Project Pumping (CVP). The Cross-Channel gate position (DXC) was also used. Each individual component was an input along with previous seven days and every week's weekly averaged value prior to that, making for a memory of 78 days for most locations except Clifton court Forebay, where the memory was extended to 113 days for better performance results.

DSM and ANN Carriage Water Demonstrations

Figure 9-1 illustrates the increase in salinity predicted by the DSM model when increasing Sacramento River flow and exports by the same amount. Figure 9-2 illustrates the increase in salinity predicted by the ANN model when increasing Sacramento River flow and exports by the same amount.

Results

The neural network model and DSM shows that carriage water (additional water needed to maintain salinity levels during increased pumping) is needed for certain locations under certain conditions. The amount required is probably smaller than previous estimates. Further work will have to be done to quantify this amount. The change in salinity with change in inputs has a transient response due to the memory of the system. This transient response may show positive and negative carriage water and may be different from the final steady–state carriage water.

Future Directions

Replacement of Minimum Delta Outflow with ANNs. ANNs will replace the MDO with a more accurate and more conceptually sound salinity simulator. The final product required by DWRSIM is the SAC flow given the other flows and salinity standard. Further work needs to be done to reverse the ANN or train a new one to predict SAC flow given the other flow conditions, gate positions, and salinity requirements.

The G–model is an improvement over MDO but it conceptually lacks the ability to investigate carriage water. This is because the G–model salinity predictions are based on one lumped parameter, the NDO. Thus if exports and Sacramento River flow are changed by the same amount, the NDO does not change, which in turn implies that the salinity prediction by the G-model does not change. Also, due to its lack of flexibility it cannot say anything about gate positions, their effect and importance. All these objections are overcome by the ANNs; thus the ANNs would be a better tool for investigating carriage water and quantifying it.

Real-Time Prediction of Salinity. An extension of the above described daily time–step salinity ANN model will be used for prediction of salinity. This will be used by DWR's

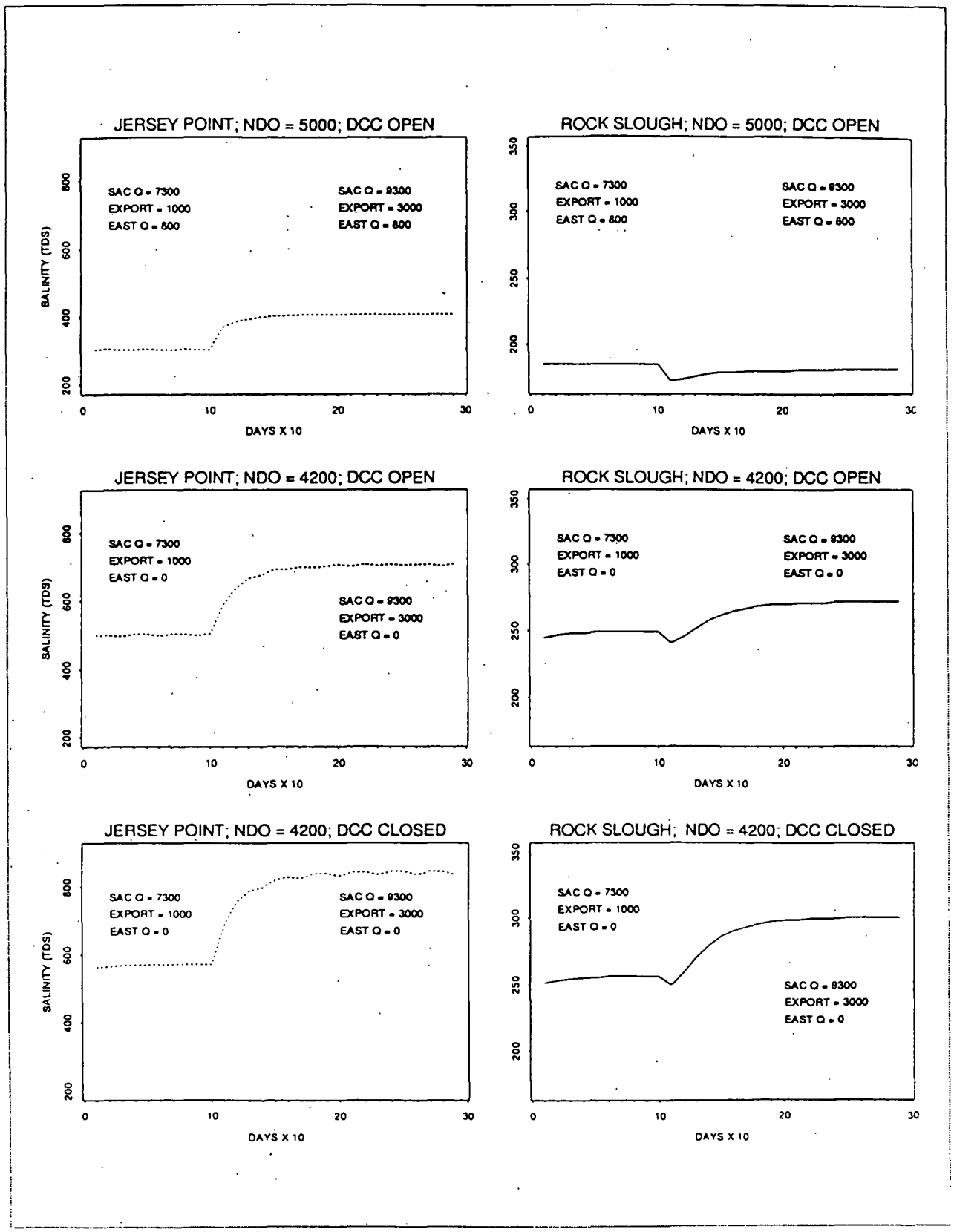

Figure 9-1. Change in Salinity When Increasing Sacramento River Flow and Exports by the Same Amount (DSM Model Run)

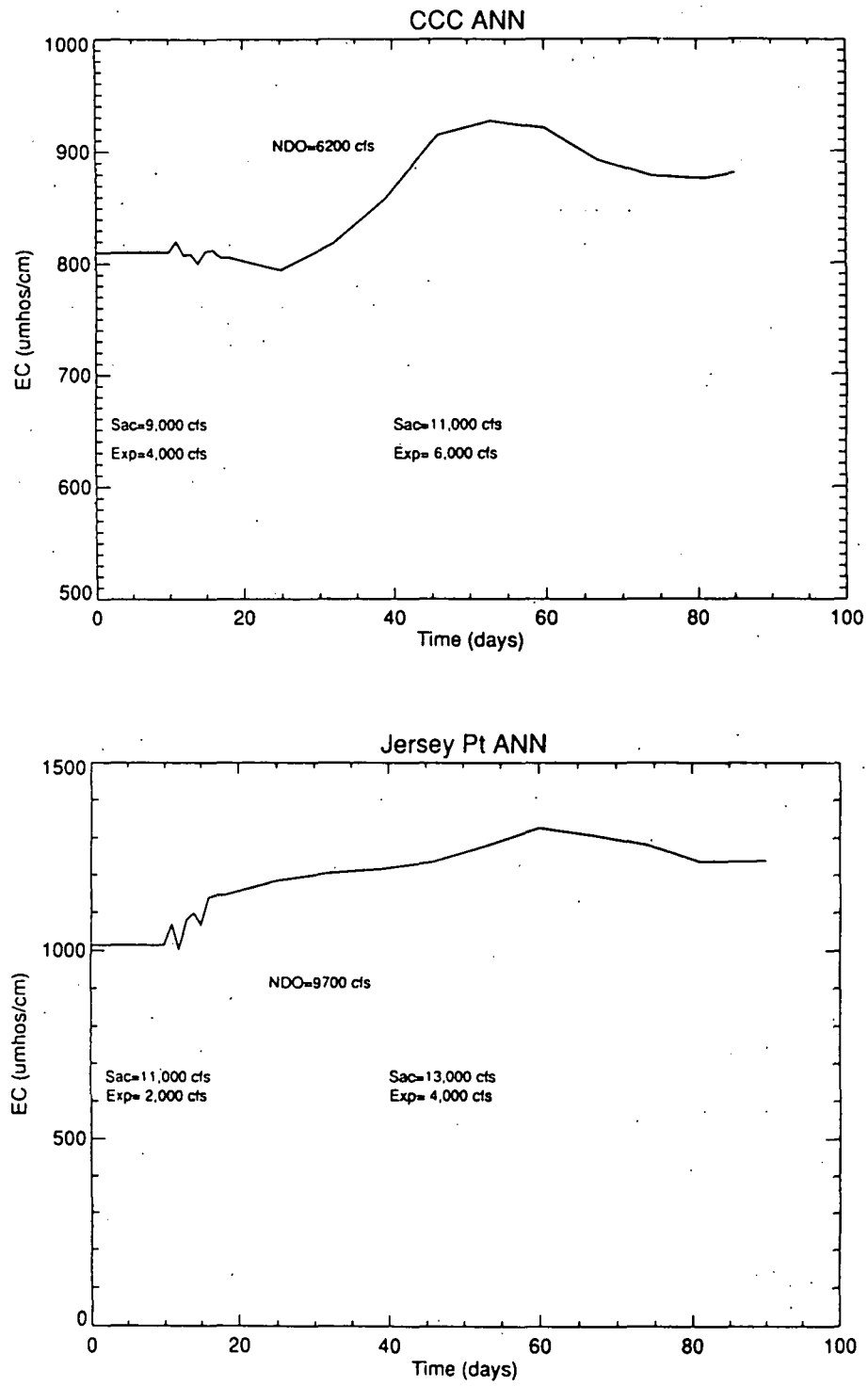

Figure 9-2. Change in Salinity When Increasing Sacramento River Flow and Exports by the Same Amount (ANN Model Run)

Operations and Maintenance division for estimating salinity in the Delta for various scenarios. Stage difference and Stage will be used as inputs to get the effect of filling and draining of the Delta. Wind and barometric pressures may be used to incorporate their effect on salinity changes in the Delta. Data depicting history of salinity may also be used as an input to further enhance the accuracy of the model.