Methodology for Flow and Salinity Estimates in the Sacramento-San Joaquin Delta and Suisun Marsh

16th Annual Progress Report
June 1995

Chapter 8:
Disinfection By-Product Formation

Authors: Paul Hutton and Nicky Sandhu

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 fuction 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.

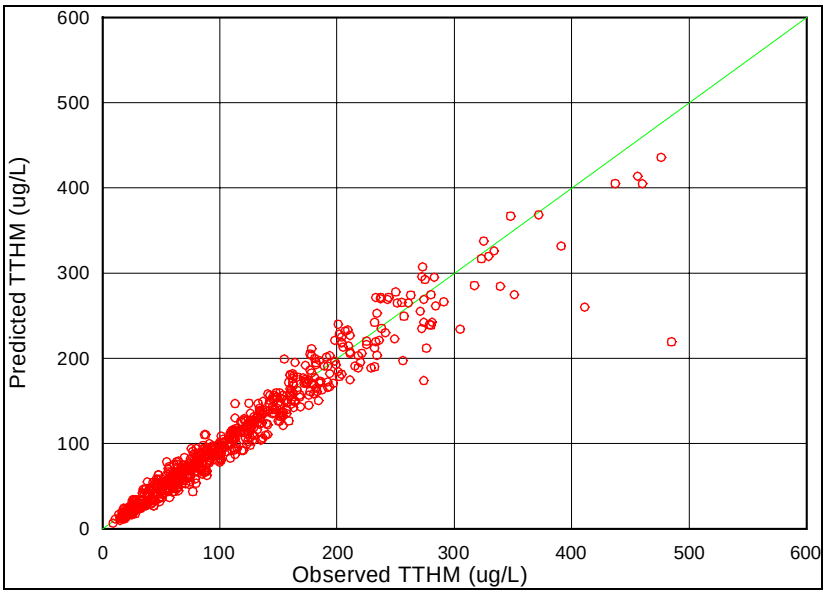

Figure 8-1: TTHM ANN: Calibration Results

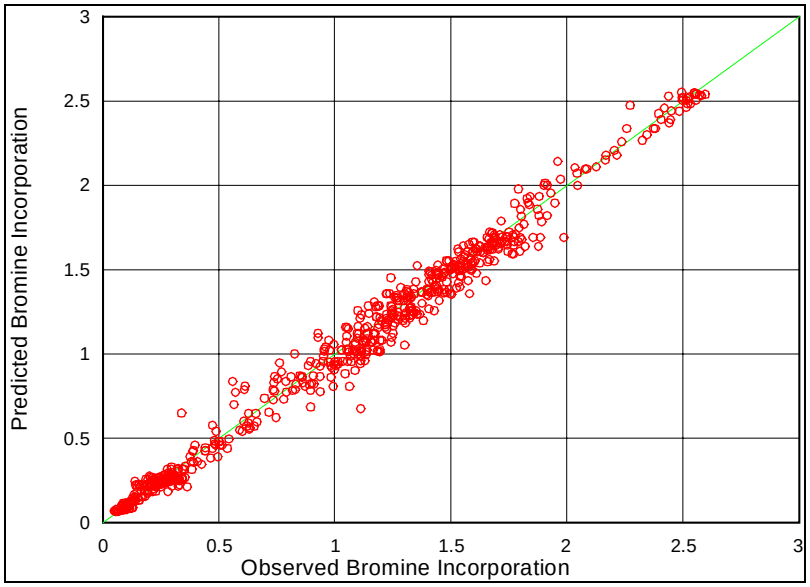

Figure 8-2: Bromine Incorporation Factor ANN: Calibration Results

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% of observed values 72% of the time for chloroform, 83% of the time for dichlorobromomethane, 88% of the time for chlorodibromomethane, and 93% 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% of observed values 92% of the time and gives predictions within ±10% of observed values 64% 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 network performance in predicting TTHM and bromine incorporation factor.

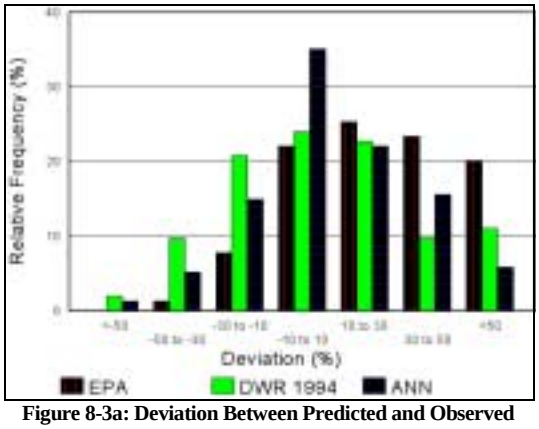

Figure 8-3a: Deviation Between Predicted and Observed Chloroform Concentrations: Validation Results

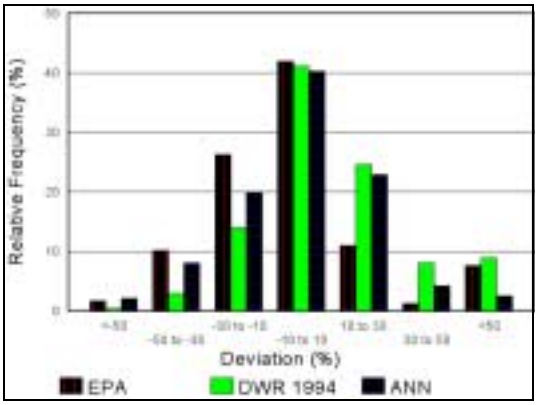

Figure 8-3b: Deviation Between Predicted and Observed Dichlorobromethane Concentrations: Validation Results

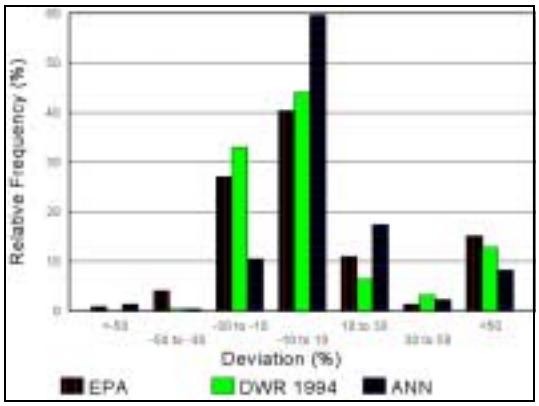

Figure 8-3c: Deviation Between Predicted and Observed Chlorodibromomethane Concentrations: Validation Results

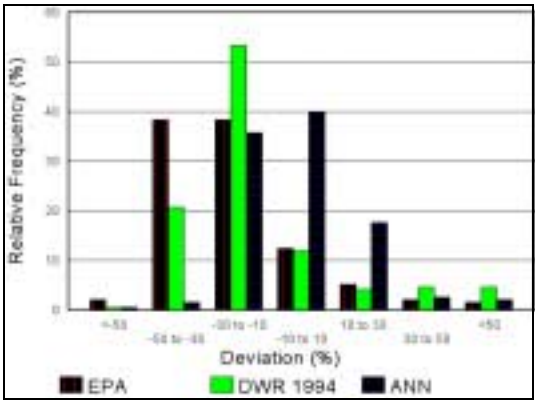

Figure 8-3d: Deviation Between Predicted and Observed Bromoform Concentrations: Validation Results

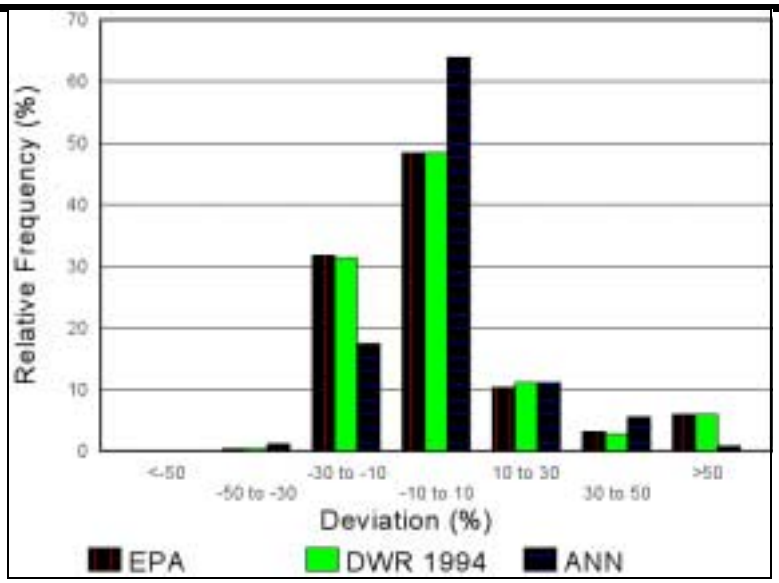

Figure 8-4: Deviation Between Predicted and Observed Total THM Concentrations: Validation Results

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% of observed values 55 to 56% of the time for chloroform and bromoform and 78 to 79% of the time for the remaining species. The EPA formulation gives TTHM predictions within ±30% of observed values 90% of the time and gives predictions within ±10% of observed values 48% of the time.

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.

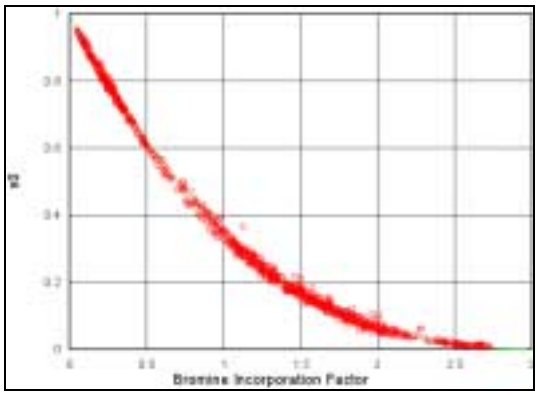

Figure 8-5a: Predicted and Observed S0 as a Function of Bromine Incorporation Factor: Calibration and Validation Data.

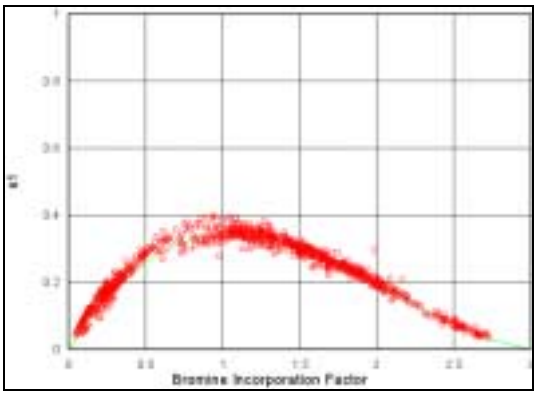

Figure 8-5b: Predicted and Observed S_1 as a Function of Bromine Incorporation Factor: Calibration and Validation Data.

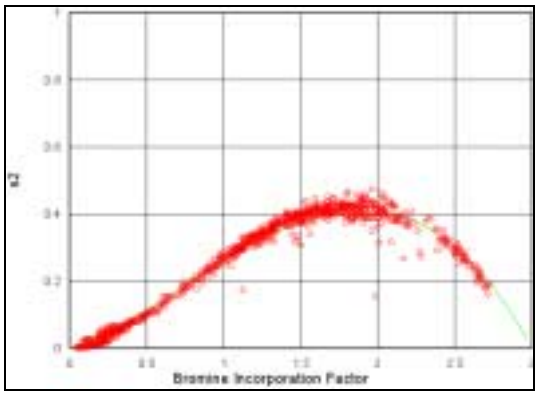

Figure 8-5c: Predicted and Observed S2 as a Function of Bromine Incorporation Factor: Calibration and Validation Data.

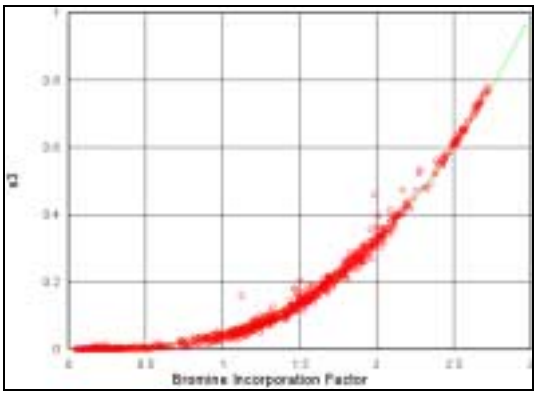

Figure 8-5d: Predicted and Observed S_3 as a Function of Bromine Incorporation Factor: Calibration and Validation Data.

References

Bay-Delta Water Quality Modeling (1993). Metropolitan Water District of Southern California, Los Angeles, Calif., prepared by Malcolm Pirnie, Inc., December.

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

"Methodology for Flow and Salinity Estimates in the Sacramento-San Joaquin Delta and San Francisco Bay." (1994). *15th Annual Progress Report to California State Water Resour. Control Board*, California Dept. of Water Resources, Sacramento, Calif., 5.1-5.13.

U.S. Environmental Protection Agency (1992). *Water Treatment Plant Simulation Program Version 1.21 User's Manual*. Office of Groundwater and Drinking Water, Washington, D.C., June.