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# Development of a full-scale artificial neural network model for the removal of natural organic matter by enhanced coagulation

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ABSTRACT: Described is the development of a full-scale artificial neural network (ANN) model for the removal of natural organic matter (NOM) by enhanced coagulation at the Rossdale Water Treatment Plant (WTP) in Edmonton, Alberta, Canada. Few attempts have been made to develop a full-scale model of the enhanced coagulation process due to extreme variability in the process parameters and the complex nonlinear relationships between them. When applied to previously unseen data, the model predicted effluent colour with a high degree of accuracy. The model will be incorporated into real-time process control at the WTP following a period of online testing.

## INTRODUCTION

As water treatment regulations for the removal of organic, biological, and other contaminants become more stringent, water utilities must actively seek out new technologies that improve treatment process control. In the water treatment industry, each process is governed by complex nonlinear relationships between numerous physical, chemical, and operational parameters. Historically, attempts have been made to model these relationships by fitting bench-scale data to mathematical formulae. Such attempts have generally been unable to account for the simultaneous change in more than one or two of the key process parameters, and often fail when applied to full-scale systems. As a result, current process control in the water treatment industry is not model-based, but rather relies upon a set of loosely defined heuristics in combination with the expert-knowledge of the plant operators.

In order to improve treatment processes, plant operators need tools that will allow them to select appropriate operational conditions required to achieve a desired effluent quality based on instantaneous influent water quality. One such tool is the artificial neural network (ANN), a robust artificial intelligence modelling technique which has the ability to learn trends and patterns in historical data in order to correctly classify new data. With respect to water treatment processes, the ANN modelling approach can be used to map the relationship between influent and effluent parameters, resulting in a process model that is based on full-scale operational data.

The purpose of this study is to illustrate the application of artificial neural networks to water treatment processes through the development of ANN model for natural organic matter (NOM) removal by enhanced coagulation at a large water treatment plant (WTP).

### NOM and enhanced coagulation

In conventional water treatment where chlorinated disinfectants are used, disinfection by-products (DBPs), such as trihalomethanes (THMs) and haloacetic acids (HAAs) can form by the reaction of residual chlorine with natural organic matter (NOM) in the treated water. As many DBPs are suspected to be carcinogenic, it is generally desirable to remove them from the drinking water stream. For conventional treatment facilities, removal is often best accomplished by enhanced coagulation [1]. The process involves the use of additional coagulant in clarification in order to improve the removal of disinfection by-product (DPB) precursors, namely natural organic matter [2].

With respect to current clarification process control, chemical dosing levels are adjusted on the basis of the results of jar-tests that are often performed infrequently throughout the plant operator's shift and often after clarified water quality begins to degrade. This methodology is reactive rather than proactive; dosing levels generally can not be adjusted until an upset occurs. As such, the magnitude of the upset is often magnified due to the time lag between the change in influent water quality and the chemical dosing adjustments. In addition the requirement to now determine the optimal dose for both particulate and organic removal adds significant complexity to jar testing methodologies. The optimal dosing levels determined by the bench-scale jar tests may also differ from those in full-scale operations due to the differences in the hydrodynamics of the two systems. In spite of these problems, the jar-test is widely used for determining dosing levels because there are no suitable full-scale models of the clarification process.

### Rossdale Water Treatment Plant description

The Rossdale Water Treatment Plant (WTP), owned and operated by AQUALTA, is located on the North Saskatchewan River, a major tributary in the Saskatchewan-Nelson river system, within the boundaries of the City of Edmonton. The river has its headwaters in the Canadian Rocky Mountains and flows in an easterly direction for approximately 500 km before

reaching the city. Much of the upstream watershed is uninhabited forest with little industrial or residential development, although there is a significant amount of agricultural land-use closer to the city.

The Rossdale WTP is composed of two independent treatment trains, identified as Plant 1 and Plant 2, which have a combined total capacity of approximately 275 ML/day. With respect to the clarification process equipment, each plant has one square cross-flow clarifier that is comprised of a rapid-mix chamber, three banks of tapered flocculators, and one sedimentation basin. The sedimentation basin for Plant 1 measures 35.0 m × 35.2 m × 4 m, while that for Plant 2 measures 46.4 m × 49.8 m × 4 m. Sedimentation is assisted by banks of upflow tube settlers that cover approximately 30% of the sedimentation basin area, and are mounted at the effluent end of the basin. With respect to the clarification process, the Rossdale facility practices enhanced alum coagulation with an anionic polymer coagulant aid. Powdered activated carbon (PAC) can also be added on demand in order to control severe taste and odour problems, which are especially prevalent during spring runoff.

Following clarification, the effluent is softened using lime and is recarbonated in order to adjust the pH. Disinfection occurs through the use of free-chlorine, followed by the addition of ammonia in order to ensure a chloramine residual in the distribution system. The water is fluoridated and is then allowed to settle in a stilling basin. The effluent is then filtered via mono-media (crushed-quartz) rapid sand filtration before being pumped into 100 ML on-site reservoirs.

### ANN overview

The ANN modelling technique is an artificial intelligence technique that simulates the human brain's problem solving processes. Artificial neural networks are able to extract concepts directly from historical data without the need for complex mathematical formulae or algorithms. In general, artificial neural networks can be applied to the following types of problems: pattern classification, clustering and categorisation, function approximation, prediction and forecasting, optimisation, associative memory, and process control [3]. The current study focuses on the development of an ANN model for effluent quality prediction. As such, the ensuing discussion is related directly to the use of ANNs for predictive purposes.

ANN models are comprised of interconnected arithmetic computing units, or artificial neurons, that are analogous to the biological neurons in the brain. Alone, each neuron can perform only the simplest of operations. When assembled into an interconnected network, or architecture, however, the neurons become part of a powerful modelling system. While many different architectures are possible, the single-layer or multilayer perceptron architectures, consisting of the input layer, the hidden layer(s), and the output layer, are commonly used for prediction and forecasting problems [3]. In single-layer or multilayer perceptron architectures, each neuron is connected to every neuron in adjacent layers by a connection weight (Fig. 1).

For prediction and forecasting problems with noncategorical outputs, a supervised ANN learning approach is often followed. The aim of supervised learning is to teach the network to map a correct model output for each set of model inputs, or pattern, by developing appropriate connections between the neurons in the architecture [4]. With respect to the actual mechanism of learning, the patterns are first presented to the network individually either in sequence or in random order. In the input layer, there is one neuron for each input parameter. The model inputs that make up the pattern are scaled by these neurons from their numeric range into a smaller and more efficient range according to a predefined scaling function. The resulting output from each input-layer neuron is multiplied by the appropriate connection weight and is transferred to each of the hidden-layer neurons. Each of the hidden-layer neurons then sums all of the inputs that it receives from the input layer. This sum is mapped into an output value according to a predefined activation function. The outputs from each of the hidden layer neurons are multiplied by the appropriate connection weight and the resulting signals are transferred to the next layer. In multiple-layer architectures, the next layer is another hidden layer and the signal is processed in the same manner as that for the first hidden layer. In single-layer architectures, the next layer is the output layer. In the output layer, there is one neuron for each output parameter. Each of these neurons sums the weighted signals from the previous hidden layer. This sum is mapped into an output value according to a predefined activation function. The output signal from each neuron is

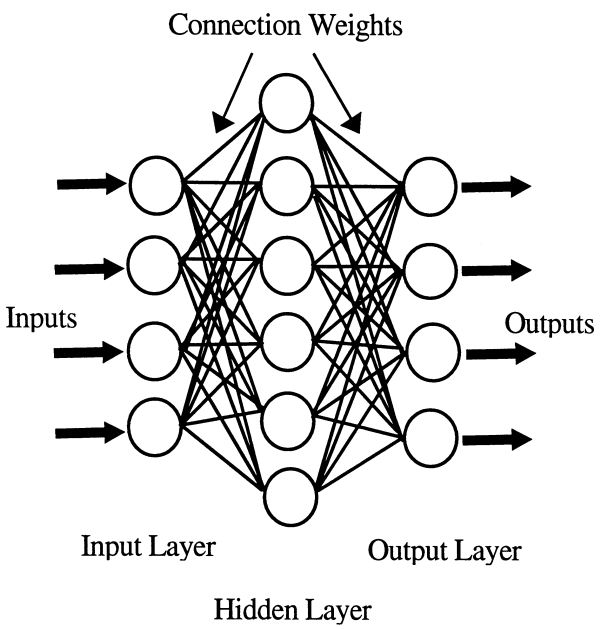


**Fig. 1** Sample ANN architecture.

then processed by the inverse of the scaling function used in the input layer in order to obtain an output value in the appropriate numeric range. This value, which is the model predicted value, is compared to the correct value for the given patterns and the connection weights are modified to decrease the sum of squared error according to a preselected learning algorithm. The entire process is repeated until the ANN produces a sufficiently small error on a previously unseen data set [5].

## MATERIALS AND METHODS

### ANN model development

The artificial neural network modelling process involves three distinct stages: source data analysis, preliminary model development, and model optimisation.

The primary objectives of the source data analysis are to gain a familiarity with the study domain and to examine the applicability of available data for model development. Initially, the problem domain must be thoroughly examined, since the blind application of the ANN technique to problems that have not been thoroughly studied will lead to the development of models with poor generalisation capabilities. Following the domain study, all the available pertinent data are examined and subjected to comprehensive statistical analyses in order to determine the range, seasonal and daily trends, and other important data characteristics. Based on the results of the data analysis, the size and range of the data set to be used in model development are selected.

The objective of the preliminary model design stage is to design and evaluate a series of network architectures that, when optimised, can be used as an effective process model. This objective is best met through the use of a four-step scheme which includes the selection of input and output parameters, the organisation of the data patterns, the selection of initial factors and levels of analysis, and the evaluation of potential architectures. With respect to the selection of input and output parameters, the output parameter which best represents the process is selected. In general, only one output parameter is selected as single-output models are generally more accurate than multiple-output models. Each input parameter is selected based on data availability and the likelihood of there being a cause-effect relationship between it and the output parameter. Once the model parameters are selected, the data patterns are selected to reflect the availability of the data. Incomplete patterns, as well as those that appear to be inconsistent with the remaining data, are removed.

The data are initially organised into two categories based on the value of the output parameter. The boundary is selected according to process performance criteria and separates regular operating conditions from process upset or special case conditions. In order to develop a successful model, the data must be further divided into three fractions: the training set, the test set, and the production set. The training set consists of data patterns that the network processes repeatedly in order to learn trends and patterns in the data. During the learning process, the network is periodically evaluated using the test set patterns in order to ensure that the network is not simply memorising the training data. The trained network is applied to the production set which consists of data that the network has never 'seen' before in order to asses the performance of the model. Each of these data sets contains an equal percentage of special case data in order to ensure that the model is trained, tested, and evaluated over a similar range of effluent quality.

In designing the initial architectures, many factors need to be considered including the type of architecture, the number of layers, the number of neurons in each layer, the type of scaling and activation functions, and the learning approach. In order to determine the optimal levels of each of these factors, the factorial experimental design approach is applied. This statistical method is used for studying the effects of varying the levels of multiple parameters in a limited number of runs. For an in-depth discussion on the mechanisms of factorial-design experimentation, please refer to the text by Box & Hunter [6].

In order to assess the model's performance, two separate statistical indicators are applied to the production data set. The $R^2$ value compares the accuracy of the model to the accuracy of a trivial benchmark model wherein the prediction is just the mean of all the samples. A perfect fit would result in an $R^2$ value of 1, a very good fit near 1, and a very poor fit near 0. The $R^2$ indicator is applied to the entire production data set and therefore serves as a measure of the model's performance in periods of routine operation as well as during special-case scenarios. The second statistical indicator, the average absolute error, is used to compare the actual process outputs with the network predictions. This indicator can serve to highlight inconsistencies in model predictions and can also be used to determine whether the model predictions are adequate for process control.

In the model optimisation stage, the most promising candidate models are optimised through the fine-tuning of the network architectures in order to minimise the error on the production set data. The optimal model will be able to follow daily trends in plant operations in addition to predicting the special case patterns. In addition the model should produce consistent results for all three data sets. The model should also be insensitive to retraining following a swapping of the testing and production sets. Finally, a plot of the model residuals should be free of obvious trends.

### Data handling and software

Three years of daily water quality and operational data, from 1994 to 1996, were used in the development of the ANN model for the Rossdale WTP. The model described here is for Plant 1. All data was obtained from AQUALTA, the water utility that oversees the operation of the Rossdale facility. Influent water

quality data are reported as the average daily value from laboratory analyses. Operational and chemical dosing levels are also reported as daily averages. All neural network model development was performed using NeuroShell v.2.0 software from Ward Systems Group Inc. of Frederick, MD.

## RESULTS AND DISCUSSION

### Source data analysis

Due to substantial seasonal variations in the North Saskatchewan River flow and ambient air temperature, the river water quality varies considerably. Raw water daily average turbidities range from approximately 2 NTU in winter, when the river is under ice cover, to over 1400 NTU during spring thaw (Table 1). Similarly, raw water colour ranges from approximately 2 TCU to 80 TCU throughout the year. The seasonal nature of these parameters is presented graphically in Figs 2 and 3.

With respect to the operating conditions at the WTP, the mean flow through Plant 1 is approximately 61 ML/day (Table 2). With respect to the alum dose, the range for both plants is from 9 mg/L under the most favourable water quality conditions, to 164 mg/L for poor quality source water. PAC is used extensively during spring runoff in order to remove taste and odour causing compounds. Doses of up to 146 mg/L have been used, although the dose exceeds 45 mg/L less than 5% of the time (Table 2). The anionic polymer dose is typically 0.30 mg/L, although higher doses may be added during periods of high alum use.

With respect to clarifier effluent parameters, the mean value for turbidity is 2.5 NTU for Plant 1 (Table 3). The effluent turbidity does not show any seasonal variations, as isolated cases of high effluent turbidity occur throughout the year. Turbidity removal, on a percentage basis, is seasonally correlated. The best removals typically occur during the spring and summer months, when influent turbidities are moderate to high. The lowest removals occur when the source water is under ice-cover and influent turbidities approach 2 NTU.

**Table 1** Rossdale WTP, data analysis for raw water quality parameters

| | | | | | Percentile | | |
|---|---|---|---|---|---|---|---|
| Parameter | Year | Mean | Min. | Max. | Range | 95% | 5% |
| pH | 1992–96 | 8.2 | 7.8 | 8.8 | 1.0 | 8.5 | 7.9 |
| Temperature (°C) | 1992–96 | 10.3 | 0.5 | 25.0 | 24.5 | 20.7 | 1.0 |
| Air temperature (°C, at 12:00 p.m.) | 1992–96 | 6.4 | −35.0 | 30.0 | 65.0 | 23.0 | −18.0 |
| River flow ($m^3/s$) | 1992–96 | 190.4 | 30.0 | 1050.0 | 1032.0 | 368.6 | 95.0 |
| Turbidity, daily high (NTU) | 1992–96 | 49.68 | 2.0 | 2400.0 | 2398.0 | 170.0 | 3.0 |
| Turbidity, daily average (NTU) | 1992–96 | 31.7 | 1.6 | 1481.0 | 1479.4 | 116.2 | 2.4 |
| Colour, daily high (TCU) | 1992–96 | 10.2 | 2.0 | 82.0 | 80.0 | 32.0 | 3.0 |
| Colour, daily average (TCU) | 1992–96 | 9.0 | 2.0 | 77.0 | 75.0 | 6.0 | 2.0 |
| Total hardness (mg/L as $CaCO_3$) | 1992–96 | 166.9 | 104.0 | 204.0 | 100.0 | 188.0 | 144.0 |
| Total alkalinity (mg/L) | 1992–96 | 133.7 | 94.0 | 174.0 | 80.0 | 149.0 | 119.0 |

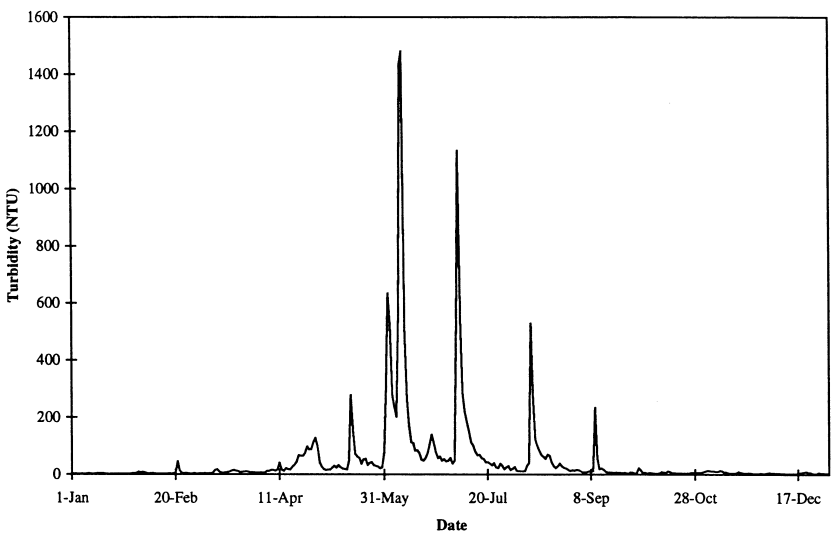


**Fig. 2** Rossdale WTP, influent daily average turbidity, 1995.

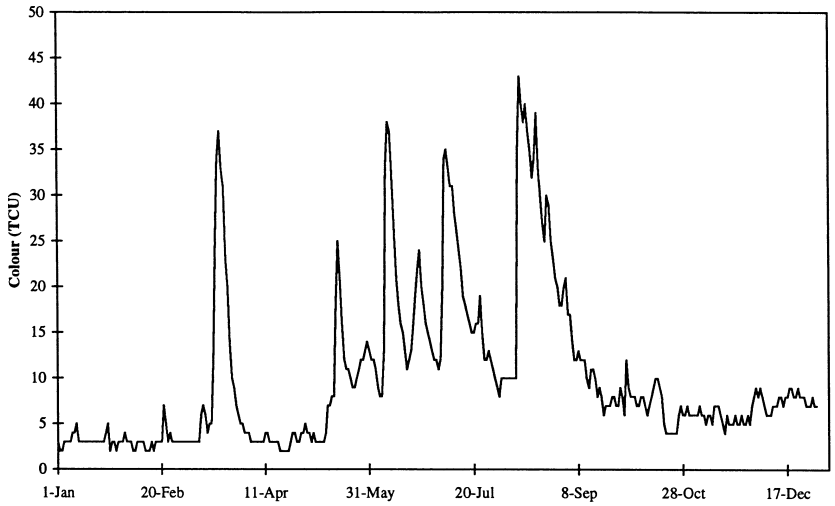


**Fig. 3** Rossdale WTP, influent daily average colour, 1995.

**Table 2** Rossdale WTP, data analysis for process parameters

| | | | | | Percentile | |
|---|---|---|---|---|---|---|
| Parameter | Dates | Mean | Min. | Max. | Range | 95% | 5% |
| Raw flow, Plant 1 (ML/day) | 1992–96 | 61.2 | 0.0 | 125.0 | 125.0 | 97.6 | 0.0 |
| Alum dose, Plant 1 (mg/L) | 1992–96 | 31.8 | 9.0 | 164.0 | 155.0 | 71.1 | 15.0 |
| PAC dose, Plant 1 (mg/L) | 1992–96 | 10.7 | 0.0 | 145.6 | 145.6 | 46.0 | 0.0 |
| Polymer dose, Plant 1 (mg/L) | 1992–96 | 0.29 | 0.00 | 0.87 | 0.87 | 0.51 | 0.00 |

**Table 3** Rossdale WTP, data analysis for clarifier effluent parameters

| | | | | | | Percentile | |
|---|---|---|---|---|---|---|---|
| Parameter | Dates | Mean | Min. | Max. | Range | 95% | 5% |
| Effluent turbidity, Plant 1 (NTU) | 1992–96 | 2.5 | 0.4 | 11.6 | 11.2 | 4.8 | 1.0 |
| Turbidity removal, Plant 1 (%) | 1992–96 | 61.6 | −129.4 | 99.9 | 229.3 | 98.4 | −3.5 |
| Effluent colour, Plant 1 (TCU) | 1992–96 | 2.1 | 0.5 | 7.4 | 6.9 | 3.8 | 1.0 |
| Colour removal, Plant 1 (%) | 1992–96 | 61.7 | −221.9 | 98.7 | 320.6 | 92.0 | 25.0 |

Under such conditions, it is sometimes possible for turbidity to increase through the treatment processes, resulting in negative removals of turbidity. Similar trends are observed for effluent colour and colour removal, although negative removals of colour are seldom observed.

### Preliminary model development

In order to select appropriate input and output parameters for the model, the study domain must be thoroughly examined. From recent literature in the areas of disinfection by-products and enhanced coagulation, over 30 potential model input parameters, as well as a number of potential outputs were identified. From these, 12 parameters were selected and grouped according to their source (Table 4). The water quality parameters provide a general indication of the quality of the WTP source water. The operational parameters are those that can be readily controlled by the plant operator and include chemical dosing levels as well as the overflow rate through the clarifiers. The lag-1 time series parameters are included as both influent turbidity and influent colour are correlated over time. With respect to the output parameter, total organic carbon (TOC), ultraviolet absorbance at a wavelength of 254 nm (UVA-254), trihalomethane formation potential (THMFP), and colour are the most common surrogate parameters used to measure NOM. From these parameters, clarifier effluent colour was selected as the model output due to the availability and reliability of colour data at the Rossdale WTP.

The entire data set consists of 889 separate days or patterns, spanning three years of water treatment at the Rossdale Water

**Table 4** Model input parameters

| Input parameter | Parameter classification |
|---|---|
| Influent turbidity | Water quality |
| Influent colour | Water quality |
| Influent pH | Water quality |
| Influent water temperature | Water quality |
| Influent alkalinity | Water quality |
| Influent hardness | Water quality |
| Alum dose | Operational |
| PAC dose | Operational |
| Polymer dose | Operational |
| Overflow rate | Operational |
| Lag 1 turbidity | Time series |
| Lag 1 colour | Time series |

Treatment Plant. The data are initially organised into two categories based on the value of the output parameter. The boundary separating the data corresponds to the 90th percentile of the clarifier effluent colour and has a numerical value of 3.20 TCU. Operationally, this value is also significant as it approximates the boundary between acceptable and poor clarifier effluent colour at the Rossdale WTP. Data for which the clarifier effluent colour exceeds 3.2 TCU falls into the special-case scenario category, while the remaining data corresponds to normal operating conditions at the WTP. The data was further divided into the training, testing, and production sets according to the method previously outlined.

For the preliminary model development stage, the effects of some of the most significant factors were evaluated using factorial design experimentation. A sample design, including factors and their corresponding initial levels of analysis, is presented in Table 5. Both the factors and the initial levels of analysis were selected based on previous experience in ANN modelling.

## Model optimisation

From the preliminary model design stage, a number of potential candidate model architectures were selected for further optimisation. Of these, the three-layer backpropagation architecture, a standard ANN architecture in which information is processed forward through the network and the prediction error is propagated backwards through the network, produced the most favourable results. When the trained network was applied to each of the data sets, the results were consistent, ranging from an $R^2$ of 0.71 for the testing set to 0.76 for the training set (Table 6). Similarly, the mean absolute error ranged from 0.30 TCU for the training set to 0.32 TCU for the testing set. In addition, when the testing and production data sets were swapped and the model was retrained and applied to the new production set, the results are identical to those for the original test set. This suggests that the internal network structure is identical for both the original and swapped data, since the original test set contains the same data patterns as the new production set. As such, the model architecture is decidedly stable, a requirement for use in process control.

The model results for previously unseen data (production data) are presented graphically in Fig. 4. The model follows the trends in the actual clarifier effluent data quite well, although two areas of apparent inaccuracy require a further examination. In the first 15 patterns, when the actual clarifier effluent colour ranges from approximately 1–2 TCU, the network tends to over-predict the actual values. From a process control standpoint however, this error is negligible since these patterns correspond to late-winter days where the raw water quality conditions are ideal and process control modifications are rarely required. With respect to the second area of concern, the model has some difficulty in predicting the highest clarifier effluent colour peaks. While the model clearly recognised that there is a peak, it tends to under-predict the actual effluent colour by approximately 1 TCU. The actual effluent colour peaks are the result of mild upsets in the clarification process, as they do not fall within the range of regular operating conditions. Since the goal of the modelling process is to develop a model that can be used in process control to avoid such upsets, it is not absolutely necessary for the model to be able to predict these peaks with complete accuracy. It is far more important that the model has good predictive capacity in the normal operating range ($<3$ TCU) of clarifier effluent colour. In this range, the model accuracy increases, with an average absolute error of only 0.28 TCU on the production set.

**Table 5** Sample factorial design, 3-layer backpropagation architecture

| Factor | − level | + level |
|---|---|---|
| Ratio of training to testing data | 1:1 | 2:1 |
| Total number of hidden layer neurons | 30 | 120 |
| Activation function | Logistic | Gaussian Compliment |

**Table 6** Model results

| Data set | $R^2$ | Mean absolute error (TCU) |
|---|---|---|
| Training | 0.76 | 0.30 |
| Testing | 0.71 | 0.32 |
| Production | 0.75 | 0.31 |
| Production (cross-test) | 0.71 | 0.32 |

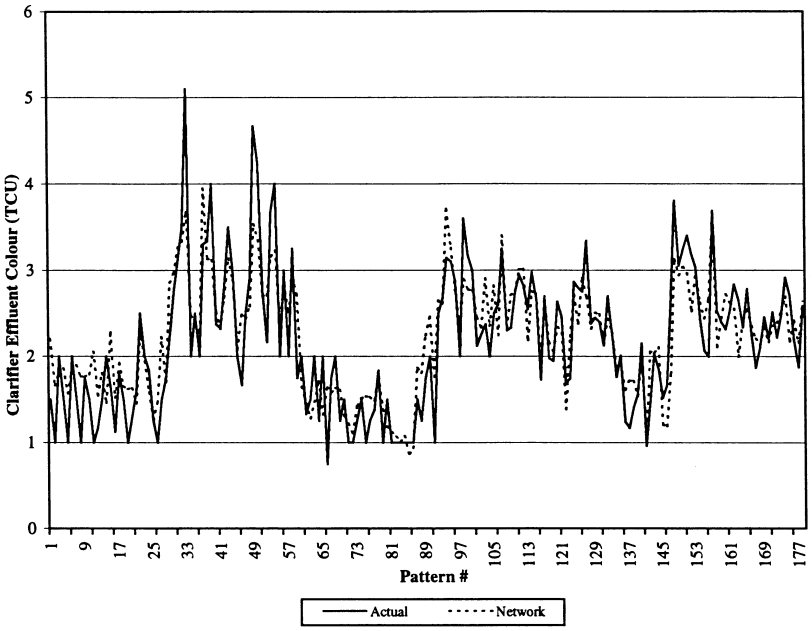


**Fig. 4** Model results for the production data set.

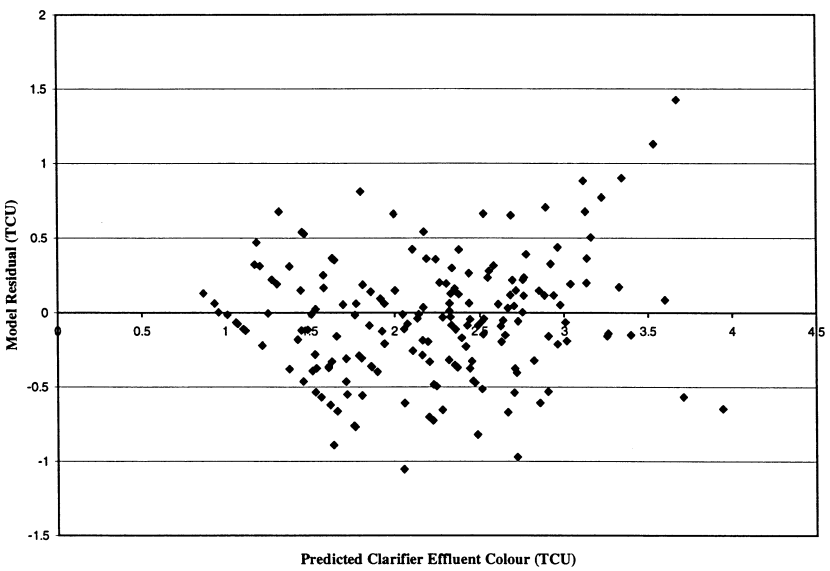


**Fig. 5** Residuals plot for the production data set.

In order to ensure that there are no obvious trends in the model residuals, a plot of the residuals across all of the patterns in the production set is presented in Fig. 5. The majority of the model residuals fall within a narrow band in the range of −0.5 TCU to 0.5 TCU. The clarifier effluent colour measurements are performed on an instrument that is only accurate to within 0.5 TCU. As such, the majority of the residuals are smaller than the instrumental error. In addition, the absolute value of the residuals exceeds 1 TCU in only three of the 178 production set patterns, suggesting that the model may be useful in process control applications.

## CONCLUSIONS

In conclusion, the artificial neural network modelling technique described above appears to hold promise for the modelling of full-scale water treatment processes. In particular, the model developed for the removal of natural organic matter by enhanced coagulation demonstrated the predictive capacity of the technique in spite of the extreme variability in the process parameters. Work is currently underway to develop models for Plant 2 at the Rossdale Water Treatment Plant as well as for the E.L. Smith Water Treatment Plant on the west side of Edmon-

ton. Following a period of on-line testing and revision, these models will be incorporated into clarification process control in order to minimise upsets in the clarification process.

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