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**PREDICTION OF PERMEATE FLUX DECLINE IN CROSSFLOW
MEMBRANE FILTRATION OF COLLOIDAL SUSPENSION: A RADIAL
BASIS FUNCTION NEURAL NETWORK APPROACH**

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Huaiqun Chen

Thesis Committee:

Albert S. Kim, Chairperson

Chittaranjan Ray

Michelle H. Teng

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ABSTRACT

The capability of a Radial Basis Function Neural Network (RBFNN) to predict long-term permeate flux decline in crossflow membrane filtration was investigated. Operating conditions such as transmembrane pressure and filtration time along with feed water parameters of particle radius, solution pH, and ionic strength were used as inputs to predict the permeate flux. Simulation results indicated that one single RBFNN accurately predicted the permeate flux decline under various experimental conditions of colloidal membrane filtrations and produced better predictability compared to those of the multiple regression method and regular multi-layer feed-forward Back Propagation Neural Network (BPNN), due to the more sophisticated training system of RBFNN. Further development of the artificial neural network approach to membrane filtration will enable the design of full or large scale processes with lab or pilot scale experiments.

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CHAPTER 1. INTRODUCTION

Compared to conventional water and wastewater treatment systems, membrane separation is a more compact operation that provides higher quality products, easier operational control and less maintenance. The major aim for efficient membrane filtration is to minimize permeate flux decline (due to membrane fouling) caused by the accumulation of particles on the membrane surface and/or within pores during filtration processes. A plethora of studies on permeate flux decline indicate that particle accumulation during crossflow colloidal membrane filtration is affected by physical and chemical characteristics of the feed water as well as hydrodynamic operating conditions (Mcdonogh et al. 1989; Romero and Davis 1990; Bacchin et al. 1996; Faibish et al. 1998).

Design and application of membrane filtration require development of predictive models that can inter-link solution properties and operating conditions to filtration performance. To predict permeate flux decline, many theoretical models have been proposed using physical, chemical, and hydrodynamic modeling parameters such as particle size, zeta potential, Hamaker constant, transmembrane pressure, solution pH, ionic strength, temperature, and so forth (Bowen and Jenner 1995). In most practical applications, effects of the concentration polarization (CP) layer are barely measurable since the cake layer is generated shortly after the CP layer forms. Thus, one of the main focuses of flux decline models is on the time-dependent changing of the cake layer

resistance during filtration while the CP layer's effect is assumed to be negligible (Romero and Davis 1988; Romero and Davis 1990; Song and M 1995; Bacchin et al. 2002).

Film theory, gel layer, osmotic pressure, and boundary layer resistance are several of the theoretical models that have been developed (Bowen and Jenner 1995). However, the accuracy of theoretical modeling has been hampered by insufficient knowledge regarding the complexity of the micro-scale phenomena occurring during the filtration processes. In addition, theoretical model designs involve specific assumptions that lead to deviations between theoretical predictions and experimental observations. Such deviations imply that fundamental, theoretical models sometimes do not have sufficient capability to depict fouling phenomena occurring in real filtration systems although the models accurately depict fundamental transport mechanisms. Purely empirical models, which can be built upon specific experimental observations and used to predict the membrane system performance, appear to be new alternatives. The multiple regression is the simplest of all the multivariate statistical techniques and can find the linear relationship between one dependent variable (output) and many independent variables (inputs) (Wilks 1995). Another popular method is the Artificial Neural Network (ANN) approach, which can obtain either linear or nonlinear relationships between inputs and output(s).

The primary advantage of ANN over theoretical models is that, as a black box model, it does not pre-require any governing equation specifically describing the underlying engineering phenomena. Instead, ANN can learn the complex transport processes of a system from given observed data, serving as an instrument for universal

data approximation. Accordingly, a considerable number of ANN applications for prediction, classification, signal processing and optimization can be found in various fields such as finance and economics, meteorology, chemistry and chemical engineering, computer science, water resources engineering, and so forth (Maas et al. 2000; Bowden et al. 2005; Bowden et al. 2005; Sahoo et al. 2005; Valverde Ramirez et al. 2005), exemplifying its great predictive potential of transport processes.

Among assorted neural networks, the multi-layer feed-forward neural network with backpropagation training algorithm, typically called backpropagation neural network (BPNN), may be one of the most widely used networks for information extraction and classification (Dornier et al. 1995; Niemi et al. 1995; Bowen et al. 1998; Chakraborty et al. 2003; Razavi et al. 2003; Shetty et al. 2003; Ramaswamy et al. 2004). However, BPNN exhibits several serious shortcomings, such as the slow convergence during its training step, susceptibility to converging to a local minimum, and inability to detect over-fitting (Schilling et al. 2001). For these aspects, the radial basis function neural network (RBFNN) seems a better alternative to BPNN as RBFNN provides easier initialization, faster training procedure and more stable performance.

Extensive research has been performed to investigate the capability of BPNN as a tool for membrane system modeling. Application of BPNN to membrane research is becoming a greatly researched topic because it has provided promising results. For example, BPNN has been harnessed to predict steady-state contaminant removal efficiency during nanofiltration in the drinking water treatment system (Shetty et al. 2003). BPNN's potential for dynamic simulation of membrane fouling during crossflow microfiltration has also been investigated (Dornier et al. 1995). Additional applications

can be found in predicting permeate flux, hydraulic resistance and rejection for various types of feed solutions (Niemi et al. 1995; Bowen et al. 1998; Chakraborty et al. 2003; Razavi et al. 2003). Moreover, BPNN's ability for classification has been shown in the development of a phenomenological model to categorize membrane pore size using the ultrasonic signal amplitude (Ramaswamy et al. 2004).

To the best of our knowledge, any RBFNN application to membrane systems has not been reported yet. The goal of this study is to study an information-integrated RBFNN applied to membrane filtration analysis and to explore its predictability of the permeate flux under various operating conditions and solution characteristics. A brief introduction to multiple regression, BPNN, and RBFNN is given, and the effectiveness of RBFNN is compared to those of multiple regression and BPNN approaches.

CHAPTER 2. REVIEW OF LITERATURE

2.1 Membrane Filtration

2.1.1 Membrane Types By Pore Size

Membrane filtration is one of the most widely used separation techniques. Depending on membrane porosity, the overall pressure-driven membrane process can be classified as microfiltration (MF), ultrafiltration (UF), nanofiltration (NF), and reversed osmosis (RO) in decreasing membrane pore size (Mallevialle et al. 1996; Mulder 1997). However, the underlying principles governing rejection of contaminant by the membrane substantially differ.

MF membranes, with pore sizes typically between 0.1 μm and 10 μm , are generally used for clarification and removal of micro-particulates. Rejection of contaminants by the MF membranes is due entirely to physical sieving of the material at the membrane surface. UF and NF membranes may reject contaminants based on a combination of physical sieving and contaminant-membrane chemistries. UF membranes, with pore sizes between 0.001 and 0.1 μm , are used for concentrating and desalting macromolecules. NF (pore size between 1 and 10 nm) and RO (pore size less than 1 nm) membranes are typically used to remove low molecular weight solutes and salt ions, respectively. Rejection of contaminants by RO membranes largely depends on the differences in solubility and diffusivity (Mallevialle et al. 1996; Mulder 1997).

2.1.2 Membrane Filtration By Operation

Based on the flow direction with respect to the membrane surface, membrane filtration processes can be generally classified into two categories: 1) deadend filtration, also known as “direct flow filtration”, and 2) crossflow filtration, also known as “tangential flow filtration” (Fig. 1).

The feed flow direction of the deadend filtration is perpendicular to the membrane surface, and so 100% of feed fluid attempts to pass through the membrane, while suspended particles with sizes greater than that of the membrane pores are blocked. Deadend filtration is not of practical interest because of its rapid flux decline stemming from continuing particle deposition on the membrane surface. In contrast, crossflow filtration is commonly employed in large-scale, industrial membrane filtration because the feed solution flows parallel to the membrane surface; one portion passes through the membrane pores (permeate) while the remainder is disposed of and/or re-circulated to the feed reservoir. The tangential feed flow over the membrane surfaces enables suspended solids to be carried downstream using shear forces that significantly reduce particle accumulation on the membrane.

2.1.3 Membrane Fouling

The major aim for efficient membrane filtration is to minimize permeate flux decline (due to membrane fouling) caused by the accumulation of particles on the surface and/or within pores of the membrane during filtration processes. Fouling is an unavoidable, deleterious phenomenon in membrane filtration that causes serious

permeate flux decline as well as deterioration of permeate quality. Particle deposition on the membrane surface can be typically classified into two processes: 1) concentration polarization (CP) and 2) cake layer formation between the CP layer and the membrane surface.

The solute concentration of the bulk phase is almost identical to that of the feed water (Fig. 1). As solute (i.e. particles in this study) transporting from a bulk phase to and retained on the membrane surface, the solute concentration above the membrane surface is higher than that of the bulk phase. This layer is called the CP layer. The solute CP layer reaches its steady state after a short time period after the filtration process begins. Thereafter, suspended particles continuously accumulate on the membrane surface and form a dense cake layer which contributes to the major resistance of the permeate water flux (Mallevialle et al. 1996; Mulder 1997).

2.1.4 Parameters

Permeate flux (J) is defined as the volume of permeate per unit membrane surface per unit time (Mallevialle et al. 1996). The permeate flux from a membrane system decreases with time (t), and eventually reaches a steady state, which is known as limiting flux. Various parameters can be modified to optimize the permeate flux during membrane filtration. In the following subsections, the definitions and effects of the four major physiochemical parameters are explained.

2.1.4.1 Transmembrane Pressure (ΔP)

Transmembrane pressure is the driving force of membrane separation, defined as the pressure difference between the filtrate and the permeate sides of the membrane (Kim 2004). In general, an increase in the transmembrane pressure monotonously enhances the flux across the membrane. The exception to this generalization occurs if a compressible cake layer is present on the surface of the membrane, where the increased transmembrane pressure can compress the pre-built cake layer, leading only to a slight increase in the permeate flux.

2.1.4.2 Solution pH

Solution pH value is an indicator of the molar concentration of hydrogen ions in solution (Mulder 1997; Kim 2004). In general, a lower permeate flux is associated with low solution pH due to the decrease in the apparent viscosity of permeating solution near the negatively-charged membrane pores. The influence of membrane pores on the liquid viscosity can be explained by the so-called electroviscous effect, which is less pronounced at higher ionic strength or near capillary surface of zero charge. At high ionic strength or low surface charge, the solution appears to exhibit a reduced viscosity when compared with the flow at low ionic strength and high surface charge.

2.1.4.3 Ionic Strength (IS)

Ionic strength is a measure of the composite effect of all ions in the feed solution, defined as half of the total sum of the concentration of all the ionic species in the solution multiplied by the square of their charge. The inter-particle distance in the cake layer

decreases at higher ionic strengths due to the decrease in the electrostatic double layer repulsive force. Consequently, a solid-packed cake layer promotes the resistance to permeate flux (Mulder 1997).

2.1.4.4 Particle Size (PS)

The suspended particle size in our study is represented by particle diameter. When larger particles are used to make the cake layer, they tend to pack with larger pores among adjacent particles, providing easier pathways for water to penetrate the layer. Changes in particle size obviously affect interparticle interactions due to more repulsive or attractive pair-wise forces, depending on the zeta potential and Hamker constant of particles, as well as ionic strength of the feed solution. However, variation in volume fraction of a cake layer due to particles size changes would not be more important than actual pore size increase, which contributes significantly less hydraulic resistance (Kim 2004).

2.2 Methodologies

2.2.1 Multiple Regression

Using a multiple regression is the simplest method to obtain the relationship between a continuous output ($\hat{y}$) and several inputs (Wilks 1995). Mathematically, multiple regression is a straightforward generalization of simple linear regression. There are k independent inputs, x_1 , x_2 , x_3 and so on up to x_k . Predicted values from multiple regression are linear combinations of the predictor variables. Therefore, the general form of a prediction equation from the multiple regression is

$$\hat{y} = a_0 + a_1x_1 + a_2x_2 + \dots + a_kx_k \quad (2.1)$$

where a_1 is the coefficient of x_1 , a_2 is the coefficient of x_2 , and so forth. The coefficient of each independent variable indicates what relationship that variable has with the dependent variable $\hat{y}$, when all the other independent variables are held constant. Multiple regression solves for unknown coefficients $a_0, a_1, a_2, \dots, a_k$ by performing a least squares fit, which generally aims to minimize the sum of the squared deviation of the observed values given the dependent variable from those predicted by the model. The least square estimator (LSE) has the following form:

$$LSE = \sum_{i=1}^n (y_i - \hat{y})^2 \quad (2.2)$$

where y is the observed dependent variable.

2.2.2 Artificial Neural Network

2.2.2.1 Introduction of ANN

Artificial Neural Network (ANN) is a parallel-distributed information-processing system (ASCE 2000) with a large number of neurons and synapses (inter-neuron connections), which is inspired by biological systems such as the human brain. It is estimated that the human brain contains over 100 billion neurons and 10^{14} inter-neuron connections. Neurons and synapses constitute the key elements for neural information processing, forming a neural network. Scientists construct a numerical model, called an artificial neural network, based on the structure and behavior of the biological neural network.

How neurons interact is different for different neurons. Generally speaking, a neuron sends its output to other neurons. Neurons' synapses collect signals by summing

all the excitatory and inhibitory influences acting on it, which is represented by a simple threshold function known as transfer function or activation function in an ANN model.

As a numerical model, the uniqueness of ANN lies in its ability to learn and generate interrelationships between the input and output of observed or experimental data without requiring any postulates and assumptions. ANNs can be classified into different categories by their network architecture, activation or transfer function, and training algorithm (Fausett 1994). A neural network's architecture defines the number of neurons and layers within the network. Training is the learning process by which an ANN calculates the interrelationship between inputs and output(s) from examples, and an optimal training algorithm could speed up the training procedure.

Generally, neurons in ANN are arranged in input, hidden and output layers. The neurons are then linked to others with associated weights and biases, which will be adjusted to optimal values during the training. The Neural Network Toolbox available in MATLAB (Mathworks, Inc., Natwick, MA) (Demuth and Beale 2003) was used to design, train and simulate the BPNN and RBFNN in this study. Later, the two neural networks are compared in terms of their performance.

2.2.2.2 Backpropagation Neural Network

The multiplayer feed-forward BPNN is one of the most widely employed ANN models in membrane study. The term “backpropagation” refers to the way in which the gradient is computed for nonlinear multiplayer networks. The BPNN usually can have multiple hidden layers, besides the input and output layers (Fig. 2). The input and output layers serve as nodes to buffer input and output for the model, respectively. Hidden

layers provide a means for relating input and output. Before running the model, weights for the neurons are randomly assigned, which makes the network much like a newborn's brain, developed but without knowledge. When training the network, once the model prediction is given, it is compared to the actual data. The adjustment based on the error between the predicted and measured data is then "backpropagated" through the network, which causes the weight adjustment. The modification of weights is done by pointing the error to the local minimum. Unfortunately, the local minimum is not always the global minimum, which will cause the model to settle in a non-optimal configuration. This is the major weakness of BPNN. More introductory overviews of BPNN can be found in several studies (Dornier et al. 1995; Niemi et al. 1995; Bowen et al. 1998; Chakraborty et al. 2003; Razavi et al. 2003; Shetty et al. 2003; Ramaswamy et al. 2004).

A transfer function is the equation computing the output of a node in a hidden or output layer. The tan-sigmoid function is the transfer function employed in the hidden layers in this study and has the following form:

$$f(n) = \tan\left(\frac{1}{1 + e^{-n}}\right) \quad (2.3)$$

where n is the net input to the neuron, which is the sum of the products of connection weight and output value from connected neurons of the previous layer with the associated bias. This transfer function is bounded between -1 and 1 so input data are usually normalized to the same range. Neurons in the output layer receive weighted input and generate the final output using a linear transfer function:

$$\hat{y} = \sum_{i=1}^m w_i f_i(n) + b_3 \quad (2.4)$$

where $\hat{y}$ is the BPNN simulation result, w_i is the optimized connection weight determined through the training process (ASCE 2000), and b_3 is the bias in the output layer.

Training is an optimization procedure in which the network weights are adjusted in order to minimize the selected error value. The error function is function that measures the difference between the target and model predicted output, as well as the generalization ability of models. Both the mean square error (MSE) and root mean square error (RMSE) were the commonly used functions to estimate the performance of the neural network:

$$MSE = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2 \quad (2.5)$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2} \quad (2.6)$$

where y is the target output value (or observed data), $\hat{y}$ is the network simulation output, and n is the total numbers of data patterns (input and output pairs) used.

2.2.2.3 Radial Basis Function Neural Network

RBFINN is another type of neural network. Such networks generally have 3 layers, the input layer, the hidden layer with the RBF non-linearity, and the linear output layer. RBFINN can overcome some of the limitations of BPNN by using a rapid training phase, having a simple architecture, and maintaining complicated mapping abilities.

In most cases, the RBFINN simulates an aimed phenomenon by using Gaussian basis functions in the hidden layer and linear transfer functions in the output layer. The

major difference in operation between the RBFNN and BPNN exists in the hidden layer. Instead of the weighted sum of the input vector used in BPNN, the distance between the input and center, as explained below, is used in the RBFNN learning process.

The first layer of the RBFNN collects the input data. Its training process determines the number of hidden neurons, m , which can be larger than that of BPNN to achieve a certain accuracy of prediction (Demuth and Beale 2003). For each neuron in the hidden layer, the distance between the input data and the center is activated by a nonlinear radial basis function, as shown in the following equation:

$$R_i = \exp \left[-(\|x_i - c_i\| b_1)^2 \right] \quad (2.7)$$

where x_i is the input vector, and b_1 and c_i are parameters that represent the bias in the hidden layer and center vector, respectively. Each neuron in the hidden layer will produce a value between 0 and 1 according to how close the input is to the location of the center. Therefore, neurons with centers closer to inputs will have more contributions to outputs; however, if neurons have centers far away from inputs, then the outputs would be nullified. Later, the output layer neurons receive the weighted inputs from the hidden layer and produce the results by using a linear combination, which is of a similar form to that of the BPNN:

$$\hat{y} = \sum_{i=1}^m w_i R_i + b_2 \quad (2.8)$$

where $\hat{y}$ is the RBFNN simulation result, w_i is the optimized connection weight determined through the training process (ASCE 2000), and b_2 is the bias in the output layer.

Figure 3 gives an insight into the structure and working procedure of the RBFNN. The open circles are bias neurons that adjust the sensitivity of the network. The biases are controlled by a specific value, called “spread” number, and each bias is set to $0.8326/\text{spread}$ (Demuth and Beale 2003). The selected “spread” value should be large enough for neurons in the hidden layer to include the whole range of input data.

In RBFNN simulations, the proper initial choice of centers and weights should be regarded as key issues. Various methods are proposed to define the center, e.g. random selection, K-mean technique, max-min algorithms, etc. (Alldrin et al. 2004). Using the Neural Network Toolbox, we chose the weight vectors as the center parameter. Instead of being randomly generated, the initial value of weights was set as the transpose of the input vector according to the MATLAB Toolbox (Demuth and Beale 2003). Once the centers have been developed, the weights linking the hidden and output layers should be updated during the training procedure. The training procedure in the RBFNN also determines the number of hidden neurons required for the simulation. The training of RBFNN is initiated by first generating a single neuron in the hidden layer, followed by continuously adding neurons to the hidden layer one at a time.

CHAPTER 3. DATA AND MODEL SETTINGS

3.1 Experimental Data

The experimental data used in this study were adopted from a paper published by Faibish et al. (1999) [1]. Three different silica (SiO_2) particles were selected as suspended colloids for the membrane filtration experiments. These three different types of silica particles, denoted as ST-XL, PST-1, and PST-3 produced by the manufacturer (Nissan Chemicals, Tarrytown, NY), have mean particle diameters of 47, 110 and 310 nm, respectively. A negatively charged UF membrane with pore size equal to 20 nm was employed in the laboratory-scale membrane test; hence, complete rejection of suspended solids on the membrane surface was observed. The schematic diagram in Figure 4 shows the membrane test unit used in these experiments. The colloidal suspension was held in a polypropylene reservoir and fed to the inlet port of the membrane module by a peristaltic pump. The feed flow rate of suspension was measured by a flow meter connected between the pump outlet and membrane inlet. A variable reluctance differential pressure transducer measured the transmembrane pressure, controlled by a needle valve installed on the outlet side of the membrane module. By weighing permeate collected in a pre-weighted beaker, the permeate flux could be measured.

3.2 Model Inputs and Outputs

In the experimental study, the effects of solution pH, ionic strength (IS), and transmembrane pressure (ΔP) on the permeate flux (J) in crossflow membrane filtration were examined. In order to examine the effect of a particular parameter in each experiment, other parameters were fixed and the permeate flux was measured accordingly. Various other operational parameters such as particle bulk concentration, temperature, and crossflow velocity were involved. In order to reduce the complexity and improve performance of the network simulation, however, the least number of inputs were selected: particle size (PS), ionic strength (IS), solution pH, transmembrane pressure (ΔP), and elapsed time (t) of the filtration process (Appendix B and C). The IS value was expressed in logarithmic scale in the simulation due to its incongruous value (wide range of data value). The multiple regression, BPNN and RBFNN were constructed to predict the variation of permeate flux with respect to time under the above physical, chemical and hydrodynamic operation parameters.

A total of 567 data points were collected from the experiments. In order to use the minimum training set in the study, the minimum ratio of training to verification data set with satisfying results are listed, according to a trial-and-error method. Approximately 17% (96 data points) of all the experimental data were used for training (Appendix B) and obtaining the interrelationship between inputs and outputs, and the remaining 83% (471 data points) were used for model performance verification (Appendix C). As all empirical models are only able to interpolate between the application boundary conditions (Shetty et al. 2003), the training data should be

representative of the entire range of experimental conditions. Therefore, extreme values of the experimental data need to be included as part of the training set.

3.3 Model Settings

3.3.1 BP Neural Network

Among many BPNN training methods available in the MATLAB Toolbox, the Levenberg-Marquardt training algorithm was selected because of its rapid convergence rate (Demuth and Beale 2003).

Learning rate is the option to regulate the training speed. It indicates the rate of change of connection weights during training. The selection of a learning rate is of critical importance in finding the minimum error. The typical learning rate is greater than 0 and less than 1. Lower learning rates require more training iterations. While a higher learning rate allows the network to converge more rapidly, the chances of a non-optimal solution are greater. To ensure the optimal performance of BPNN, the learning rate in this study was set to 0.01.

Another option in controlling the training procedure is the number of epochs, which represents the total number of times the entire set of training data will pass through the network structure. Increasing this number will likely improve the accuracy of the model, but at the cost of time. Conversely, decreasing the number of epochs will likely lower the accuracy, but take less time. A moderately high number of epochs, 400, was assigned for this study.

During the backpropagation training, the validation of suitability of the neural network simulation was estimated by calculating the Mean Square Error (MSE) between

the observed and ANN-simulated data. In our study, the maximum number of epochs, target error goal 'MSE', and minimum performance gradient were set to 400, 10^{-10} , and 10^{-6} , respectively. Training stops when the maximum number of epochs was reached, or either the MSE or performance gradient were minimized to arrive at the pre-determined goal. Through a trial-and-error method, the optimal network structure for the current BPNN simulation was determined to have two hidden layers, one containing 4 and the other containing 2 hidden neurons as shown in Figure 2.

3.3.2 RBF Neural Network

The model setting of RBFNN is relatively easier than BPNN. Before training starts, only a few key training parameters should be assigned. In our study, the target error goal MSE and the maximum number of neurons were set to 10^{-10} and 80, respectively. Training was stopped when either of the following criteria was met: 1) MSE was minimized to be less than the pre-determined goal; 2) the maximum number of neurons was reached. Because the value of spread affects the quality of prediction, a trial-and-error method was employed, wherein several spread numbers are tested and the best one is accepted. By doing so, we found that the optimal spread number was 80.

CHAPTER 4. RESULTS AND DISCUSSIONS

Changing the physical, chemical and operating conditions is a useful technique to determine their effects on permeate flux. Experimental data, according to Faibish et al.'s paper, are divided into three sets to represent different parameters' effects on permeate flux. To ensure that the trained RBFNN can be used for prediction under various conditions, sets of six training points were selected from permeate samples in those three data sets as shown in Figs 5-8 (Appendix B). In this section, our model simulation results are presented and compared to Faibish et al.'s experimental observation.

4.1 Effect of Solution pH

In order to study the effects of pH on the permeate flux, the solution pH value was regulated by adding NaHCO_3 or NaOH to the feed solution (Faibish et al. 1998). Figures 5 and 6 show comparisons of the RBFNN predictions and the experimentally observed permeate fluxes at two pH values of the feed solution (10^{-1} and 10^{-3} M KCl). Intermittent training data, shown as $\times$, were selected from the permeate flux profile of pH 6.1 and 10.0 and then used to predict all the flux decline behaviors at pHs of 6.1, 8.3 and 10.0. The results generally depict the excellent performance of the RBF network as it accurately interpolates and reproduces the complex non-linear profiles of the transient permeate flux decline under various solution pHs and ionic strengths.

The correlation coefficient between the observed and predicted permeate flux was as high as 0.993, although minor departures were observed during the early stages of filtration, where permeate flux degenerates dramatically. The paired t-tests indicated that there was no statistical difference between the experimental values and neural network predictions at the 99% confidence level for both high (10^{-1} M) and low (10^{-3} M) ionic strengths.

Both model prediction and experimental data demonstrated that the feed water pH had only minor effects on the permeate flux. Comparing Figures 5 and 6 indicated that the initial permeate flux slightly decreased with pH and this behavior was captured by the RBFNN. However, the trained RBFNN did not accurately duplicate the almost identical permeate fluxes at pHs 8.3 and 10.0 in Figure 6. The neural network slightly over-predicted the initial permeate flux at pH 8.3 for the first 10 minutes of filtration. We think this over-prediction stemmed from preparing the training data set only from pH 6.1 and 10.0 cases, excluding pH 8.3 data.

Comparison of Figures 5 and 6 showed that initial permeate flux increases at higher ionic strength and lower pH due to the narrow capillary effect on fluid viscosity. At the initial stage, when particle deposition was negligible, the intrinsic membrane resistance dominated. Under low pH and high ionic strength conditions, the decreasing fluid viscosity near membrane pores allowed water to penetrate the membrane pores with relative ease, leading to the initial enhanced permeate flux. However, at the later stages of the membrane filtration when the cake resistance became dominant, the steady state permeate fluxes became simply independent of the solution pH.

4.2 Effect of Ionic Strength

The RBFNN's predictability of the influence of ionic strength on the permeate flux was investigated using three different particle sizes of 47 nm, 110 nm and 310 nm, and four ionic strength values of 10^{-4} , 10^{-3} , 10^{-2} , and 10^{-1} M KCl. The experimental data and the modeling results are shown in Figure 7, which clearly revealed the excellent predictability of the RBFNN for permeate flux over a wide range of ionic strengths and particle sizes. The predicted and experimental data did not show noticeable difference with correlation coefficient of 0.9944 and RMSE of 0.076 at the 99% confidence level through the entire time-dependent permeate flux.

As expected, increasing ionic strength promoted severe permeate flux decline and accelerated reaching a limiting flux level because the electrostatic double layer repulsion was mollified by the increasing ionic strength, causing a dense cake layer of enhanced hydraulic resistance. In Figures 7(a) and 7(b), the RBFNN closely captured the underlying fundamental effects of the double layer repulsion through various ionic strength on the permeate flux. On the other hand, Figure 7(c) reveals a quite different trend of transient fluxes from those of Figure 7(a) and 7(b), which seem to converge into a single limiting permeate flux level. This behavior indicated that the ratio of cake resistance to particle size can suppress the influence of interparticle interactions, leaving hydrodynamics as a dominating mechanism of flux decline. The trained RBFNN shows its ability to predict flux decline for ionic strengths of 10^{-2} and 10^{-3} M by learning two different types of underlying mechanisms, i.e. interparticle and hydrodynamic interactions.

4.3 Effect of Transmembrane Pressure

The ability of RBFNN to simulate the transmembrane pressure effect on the permeate flux is examined in this section. Results shown in Figure 8 demonstrate that RBF model can closely predict the permeate flux under different transmembrane pressures of 62.1, 41.4, and 20.7 kPa. The accuracy of the prediction is reflected by a correlation coefficient of 0.994 and RMSE of 0.092.

Figure 8 shows that the permeate flux tends to reach a converging limiting flux under the same ionic strength regardless of applied transmembrane pressure and initial flux. As expected, Figure 8 confirmed that flux decline was accelerated by increasing transmembrane pressure and ionic strength (as described in section 4.2). A higher transmembrane pressure elevated the initial permeate flux by pushing more water toward a clean membrane while the particle concentration polarization was still developing. Contrary to the gain in the initial stage, the higher transmembrane pressure at a later stage pulled more particles toward the membrane surface by providing faster permeate velocity and thus contributed to the rapid generation of the deposit cake layer which caused dramatic decline of the permeate flux. Moreover, the higher pressure significantly compressed the pre-built cake layer so that it became denser and additionally contributed to the rapid flux decline. Decreasing flux is observed when both the initial flux and ionic strength are low which reflects slow and sparse formation of the cake layer.

4.4 Performance of Multiple Regression, BPNN and RBFNN

As noted in the introduction, BPNN has been widely used in the past decade as the standard ANN method to model membrane performance (Dornier et al. 1995; Niemi

et al. 1995; Bowen et al. 1998; Chakraborty et al. 2003; Razavi et al. 2003; Shetty et al. 2003; Ramaswamy et al. 2004). This section mainly describes the superiority of RBFNN over BPNN by comparing their performances using 96 ($=N_{train}$) filtration data points for training and 471 ($=N_{test}$) points for testing out of total 567 ($=N_{total}$) points of permeate flux vs. filtration time.

Figure 9(a) summarizes the RBFNN predictions for various operational conditions in Figures 5 to 8 by plotting predicted values as a function of experimental values of identical input parameters. The solid line in Figure 9(a) represents the perfect 1:1 match of the measured and predicted values of the permeate flux, and the dotted lines depict $\pm 10\%$ relative error from the 1:1 match line. Most of data shown in Figure 9(a) are located near the 1:1 match straight line. The number of points beyond $\pm 10\%$ relative error lines, N_{10} is 14 when the number of training data set N_{test} is 471, indicating 97% of the points are located within the $\pm 10\%$ relative error. This excellent performance of RBFNN is also quantified by a RMSE of 0.082 and the variance (R^2) of 0.988. In spite of broad variations of feed water parameters and operational conditions, which cause complexity to the filtration system, the results overall indicate that employing only 17% (96 out of 567 points) of the total data for training renders satisfactory prediction of the remaining 83% (471 out of 567 points) of the data.

Previous investigations have suggested that RBFNNs have multiple advantages in comparison with the performance of BPNNs. In order to verify this concept, an undifferentiated simulation was also carried out by BPNN, and the result is presented in Figure 9(b). The hollow circles are clouded near the 1:1 match line, suggesting that BPNN is also able to accurately predict the permeate flux under different operational

status to a certain extent. However, when compared with the RBFNN prediction in Figure 9(a), BPNN produces a somehow more scattered plot compared to that of the RBFNN, and 61 ($=N_{10}$) out of 471 points are not confined within the two dotted lines. (Note that N_{10} of the RBFNN is 14.) Only 87% of the predicted points are within acceptable error whereas 97% were within $\pm 10\%$ relative error using RBFNN.

The multiple regression equation obtained from the training data has the following form:

$$\hat{J} = 0.943 + 0.025[\Delta P] + 0.1663[IS] - 0.0192[pH] + 0.0028[PS] - 0.0133[t] \quad (4.1)$$

A regression equation can also be used to predict values of the permeate flux for the remaining data. Results from multiple regression are additionally shown in Figure 9(c). It is clearly evident that, given the same information, multiple regression has a less accurate performance, mainly because the complex nonlinear membrane filtration process could not be presented by simple linear regression. Compared with Figure 9(a) and 9(b), hollow circles in Figure 9(c) are more detached from the 1:1 match line. More than half (51.6%) of the predicted points (471) were out of the $\pm 10\%$ relative error range.

Finally, Table 1 compares the performance of RBFNN, BPNN and multiple regression using four parameters - variance (R^2), RMSE, N_{10} and required simulation time. RBFNN much more closely predicts the experimental observations in comparison to BPNN and multiple regression. Additionally, the RBF training method eventually speeds up the training process of the neural network by as much as 40 times over the BPNN training rate, providing higher adaptability when a large set of observed data is used to investigate more complex filtration systems. Nevertheless, comparing the model result for one data set alone cannot prove the robust advantage of RBFNN over the permeate

flux prediction. For this reason, an supplementary case study was conducted in Appendix A to serve as the additional support of the superiority of RBFNN over BPNN and multiple regression on membrane permeate flux prediction.

Table 1. Comparison of the performance of RBFNN, BPNN and multiple regression in terms of variance (R^2), root mean square error (RMSE), number of points beyond $\pm 10\%$ relative error (N_{10}), and simulation time, given the same number of points for total data set (N_{total}), training set (N_{train}), and testing set (N_{test}).

	N_{total}	N_{train}	N_{test}	R^2	RMSE	N_{10}	Simulation time (sec)
RBFNN	567	96	471	0.988	0.082	14	2.47
BPNN	567	96	471	0.958	0.156	61	96.32
MR	567	96	471	0.755	0.332	244	0.046

CHAPTER 5. CONCLUSIONS

Due to the complex physicochemical micro-phenomena occurring during membrane filtration, conventional theoretical models have been able to predict the filtration procedure only under limited conditions and/or with specific and/or inevitable assumptions. An artificial neural network method provides a unified approach for analysis and prediction of the performance of membranes under various combinations of operational conditions. In this study, the RBF neural network was applied to predict the permeate flux on crossflow membrane filtration as a function of transmembrane pressure, ionic strength, solution pH, particle size and elapsed filtration time. Results show that the transient profiles of the permeate flux during the crossflow membrane filtration can be predicted by a single RBFNN with acute accuracy given a limited number of training data. Comparison of the performances of RBFNN, BPNN and multiple regression confirmed the superiority of the RBFNN in terms of the variance, RMSE, N_{10} and simulation time required of higher accuracy.

As a consequence, it may not be necessary to carry out an entire series of expensive pilot or full-scale tests to collect and verify filtration data. The RBFNN can interpolate the performance of membrane filtration under other conditions of interest by using widely ranged but sparse data points to reduce the time and costs required. Although pilot scale experimental tests restrict the number of operating parameters that

generally are of importance in larger scale applications, they still can closely simulate full-scale operations. In the same manner, RBFNN can also serve as potential prediction tools for full-scale operation, possibly combining several trained networks of different scales into one network.

Figure 1. Schematic diagrams of deadend and crossflow membrane filtrations.

Figure 2. Architecture of BP neural network employed in this study. BPNN inputs consist of particle size (PS), ionic strength (IS), solution pH, transmembrane pressure (ΔP), and elapsed time (t), which are used as input parameters to predict the permeate flux (J). b_1 , is the bias in the input layer; b_2 and b_3 are biases in two hidden layers.

Figure 3. Architecture of RBF neural network employed in this study. RBFNN inputs consist of particle size (PS), ionic strength (IS), solution pH, transmembrane pressure (ΔP), and elapsed time (t), which are used as input parameters to predict the permeate flux (J). b_1 and b_2 are biases in the input and hidden layer, respectively.

Figure 4. A schematic diagram of a membrane test unit. (Adopted from Faibish et al. (1998)).

Figure 5. Experimental data and ANN predictions on effect of solution pH on permeate flux decline with ionic strength of 10^{-1} M KCl. The filtration conditions employed are particle size 47 nm, transmembrane pressure 41.4 kPa (6 psi), particle volume concentration 0.01%, cross flow velocity 0.246 m/s, and temperature 20 °C. At each pH value, the solid and the hollow symbols represent experimentally observed and ANN simulated data while × indicates data points used for the training process.

Figure 6. Experimental data and ANN predictions on the effect of solution pH on permeate flux decline with ionic strength of 10^{-3} M KCl. The filtration conditions employed are particle size 47 nm, transmembrane pressure 41.4 kPa (6 psi), particle volume concentration 0.01%, cross flow velocity 0.246 m/s, and temperature 20 °C. At each pH value, the solid and the hollow symbols represent experimentally observed and ANN simulated data while $\times$ indicates data points used for the training process.

Figure 7. Experimental data and ANN predictions on the effect of ionic strength on permeate flux decline for (a) 47 nm, (b) 110 nm and (c) 310 nm particles. The filtration conditions employed were pH 10, transmembrane pressure 41.4 kPa (6 psi), particle volume concentration 0.01%, cross flow velocity 0.246 m/s, and temperature 20 °C. For each particle size, the symbol $\times$ and $+$ indicate the selected data points of ionic strength of 10^{-4} and 10^{-1} M, respectively, for the training process. The solid symbols indicate experimentally observed data of ionic strength 10^{-4} M ($\blacktriangle$), 10^{-3} M ($\blacksquare$), 10^{-2} M ($\bullet$), and 10^{-1} M ($\blacktriangledown$) of KCl while the corresponding hollow symbols represent the simulation results.

Figure 8. Experimental data and ANN predictions on the effect of transmembrane pressure on permeate flux decline for ionic strengths of (a) 10^{-4} M , (b) 10^{-3} M and (c) 10^{-2} M KCl. The filtration conditions employed were pH 10, particle size 47 nm, particle volume concentration 0.01%, cross flow velocity 0.246 m/s, and temperature 20 °C. For each particle size, the symbol $\times$ and $+$ indicate the selected data points of transmembrane pressure of 62.1 kPa (9 psi) and 20.7 kPa (3 psi), respectively, for the training process. The solid symbols indicate experimentally observed data of transmembrane pressure 62.1 kPa (9 psi) (▲), 41.4 kPa (6 psi) (●), and 20.7 kPa (3 psi) (▼) while the corresponding hollow symbols represent the simulation results.

Figure 9(a). RBFNN predictions of permeate flux with experimental measurement under different operational conditions. The solid straight line represents the line of equality and the dashed lines represent $\pm 10\%$ variance from it. The variance and RMSE between the predicted and measured data are also provided.

Figure 9(b). BPNN predictions of permeate flux with experimental measurement under different operational conditions. The solid straight line represents the line of equality and the dashed lines represent $\pm 10\%$ variance from it. The variance and RMSE between the predicted and measured data are also provided.

Figure 9(c). Multiple regression predictions of permeate flux with experimental measurement under different operational conditions. The solid straight line represents the line of equality and the dashed lines represent $\pm 10\%$ variance from it. The variance and RMSE between the predicted and measured data are also provided.

APPENDIX A. A SUPPLEMENTARY CASE STUDY

To examine whether a different ratio of data points in training and validation sets has any effect on the RBFNN's advantage, an additional case study was performed by using more training and less validation data points. Similar to the study presented in Chapter 4, a total of 567 data points from membrane experiments were used. Of these 567 data points, approximately 78% (441 data points) of all the experimental data were used for training and obtaining the interrelationship between inputs and outputs, and the remaining 22% (126 data points) were used for model performance verification. As mentioned in Chapter 3, as all empirical models are only able to interpolate between the application boundary conditions (Shetty et al. 2003), the training data should be representative of the entire range of experimental conditions. Therefore, extreme values of the experimental data need to be included as part of the training set, in order to obtain better model prediction. In addition, it is always required to provide the same quality and quantity of data in order to compare the model performance. Thus, the results presented below all employed the same training and validation data sets.

Similarity, both RBFNN and BPNN model simulation applied in this supplementary case preserve the settings used in the study. The only difference is that the optimal "spread" number for RBFNN in the current case is 24. The regression equation computed from the model has the following form:

$$\hat{J} = 0.712 + 0.024[\Delta P] + 0.195[IS] - 0.011[pH] + 0.0027[PS] - 0.012[t] \quad (A)$$

Model performance was investigated by expressing the predicted data as a function of measured data (Figs. A1, A2, and A3). RBFNN, BPNN and multiple regression all exhibited better performance by providing more training data, when compared to the results in Chapter 4. This advantage of having more training data point was more evident in the BPNN, which showed an increased R^2 from 0.958 to 0.982 and decreased RMSE from 0.156 to 0.079. In terms of the model performance, obviously, both RBFNN and BPNN produced better results than the multiple regression did, such that most of predicted data were within the $\pm 10\%$ relative error. Multiple regression still cannot fully predict the nonlinear variation of permeate flux in membrane filtration, even given more sufficient training data points. By comparing the performance parameters of RBFNN and BPNN (Table. A1), one can still notice the advantage of RBFNN. Meanwhile, the superiority of RBFNN over BPNN is considerably reduced, showing relatively close values of R^2 and RMSE.

Table A1. Comparison of the performance of RBFNN, BPNN and multiple regression for a supplementary case in terms of variance (R^2), root mean square error (RMSE), number of points beyond $\pm 10\%$ relative error (N_{10}), and simulation time, given the same number of points for total data set (N_{total}), training set (N_{train}), and testing set (N_{test}) for an additional case.

	N_{total}	N_{train}	N_{test}	R^2	RMSE	N_{10}	Simulation time (sec)
RBFNN	567	441	126	0.984	0.079	2	7.23
BPNN	567	441	126	0.982	0.085	4	97
MR	567	441	126	0.798	0.282	35	0.046

Figure A1 RBFNN predictions of permeate flux for a supplementary case. The solid straight line represents the line of equality and the dashed lines represent $\pm 10\%$ variance from it. The variance and RMSE between the predicted and measured data are also provided.

Figure A2 BPNN predictions of permeate flux for a supplementary case. The solid straight line represents the line of equality and the dashed lines represent $\pm 10\%$ variance from it. The variance and RMSE between the predicted and measured data are also provided.

Figure A3 Multiple regression predictions of permeate flux for a supplementary case. The solid straight line represents the line of equality and the dashed lines represent $\pm 10\%$ variance from it. The variance and RMSE between the predicted and measured data are also provided.

APPENDIX B. EXPERIMENTAL DATA (TRAINING SET)

NO	P	IS	pH	PS	t	J
	kPs	M		nm	min	m/s
1	41	1	6.1	47	0	3.6
2	41	1	6.1	47	22	1.1
3	41	1	6.1	47	42	1
4	41	1	6.1	47	62	0.8
5	41	1	6.1	47	85	0.7
6	41	1	6.1	47	115	0.6
7	41	1	10	47	0	3.1
8	41	1	10	47	22	1.3
9	41	1	10	47	42	1
10	41	1	10	47	62	0.9
11	41	1	10	47	85	0.8
12	41	1	10	47	115	0.7
13	41	3	6.1	47	0	3.5
14	41	3	6.1	47	22	2.2
15	41	3	6.1	47	42	1.6
16	41	3	6.1	47	62	1.5
17	41	3	6.1	47	85	1.4
18	41	3	6.1	47	115	1.3
19	41	3	10	47	0	2.6
20	41	3	10	47	22	2.1
21	41	3	10	47	42	1.7
22	41	3	10	47	62	1.5
23	41	3	10	47	85	1.4
24	41	3	10	47	115	1.3
25	41	1	10	47	0	3.1
26	41	1	10	47	22	1.3
27	41	1	10	47	42	1
28	41	1	10	47	62	0.9
29	41	1	10	47	85	0.8
30	41	1	10	47	115	0.7

NO	P	IS	pH	PS	t	J
	kPs	M		nm	min	m/s
31	41	4	10	47	0	2.6
32	41	4	10	47	22	2.3
33	41	4	10	47	42	2
34	41	4	10	47	62	1.8
35	41	4	10	47	85	1.6
36	41	4	10	47	115	1.5
37	41	1	10	110	0	3.1
38	41	1	10	110	22	1.7
39	41	1	10	110	42	1.2
40	41	1	10	110	62	1.1
41	41	1	10	110	85	0.9
42	41	1	10	110	115	0.8
43	41	4	10	110	0	2.6
44	41	4	10	110	22	2.4
45	41	4	10	110	42	2.1
46	41	4	10	110	62	1.9
47	41	4	10	110	85	1.6
48	41	4	10	110	115	1.5
49	41	1	10	310	0	3.1
50	41	1	10	310	22	2.7
51	41	1	10	310	42	2.4
52	41	1	10	310	62	2.3
53	41	1	10	310	85	2.1
54	41	1	10	310	115	2
55	41	4	10	310	0	2.6
56	41	4	10	310	22	2.5
57	41	4	10	310	42	2.4
58	41	4	10	310	62	2.2
59	41	4	10	310	85	2.1
60	41	4	10	310	115	2

Appendix B. (Continued) Experimental Data (Training Set)

NO	P	IS	pH	PS	t	J
	kPs	M		nm	min	m/s
61	62	4	10	47	0	4.3
62	62	4	10	47	22	2.8
63	62	4	10	47	42	2.2
64	62	4	10	47	62	2
65	62	4	10	47	85	1.8
66	62	4	10	47	115	1.6
67	21	4	10	47	0	1.5
68	21	4	10	47	22	1.4
69	21	4	10	47	42	1.3
70	21	4	10	47	62	1.3
71	21	4	10	47	85	1.2
72	21	4	10	47	115	1.2
73	62	3	10	47	0	4.4
74	62	3	10	47	22	2.6
75	62	3	10	47	42	2
76	62	3	10	47	62	1.7
77	62	3	10	47	85	1.6
78	62	3	10	47	115	1.5
79	21	3	10	47	0	1.4
80	21	3	10	47	22	1.3
81	21	3	10	47	42	1.2
82	21	3	10	47	62	1.2
83	21	3	10	47	85	1.2
84	21	3	10	47	115	1.1
85	62	2	10	47	0	4.7
86	62	2	10	47	22	2
87	62	2	10	47	42	1.5
88	62	2	10	47	62	1.3
89	62	2	10	47	85	1.1
90	62	2	10	47	115	1.1

NO	P	IS	pH	PS	t	J
	kPs	M		nm	min	m/s
91	21	2	10	47	0	1.5
92	21	2	10	47	22	1.1
93	21	2	10	47	42	1
94	21	2	10	47	62	0.9
95	21	2	10	47	85	0.9
96	21	2	10	47	115	0.8

APPENDIX C. EXPERIMENTAL DATA (VALIDATION SET)

NO	P	IS	pH	PS	t	J
	kPs	M		nm	min	m/s
1	41.4	1	6.1	47	2	3.08
2	41.4	1	6.1	47	7	1.97
3	41.4	1	6.1	47	12	1.47
4	41.4	1	6.1	47	17	1.25
5	41.4	1	6.1	47	27	1.08
6	41.4	1	6.1	47	32	0.95
7	41.4	1	6.1	47	37	0.9
8	41.4	1	6.1	47	47	0.87
9	41.4	1	6.1	47	52	0.78
10	41.4	1	6.1	47	57	0.77
11	41.4	1	6.1	47	67	0.72
12	41.4	1	6.1	47	72	0.71
13	41.4	1	6.1	47	77	0.7
14	41.4	1	6.1	47	95	0.67
15	41.4	1	6.1	47	105	0.65
16	41.4	1	8.3	47	0	3.35
17	41.4	1	8.3	47	2	3
18	41.4	1	8.3	47	7	2.2
19	41.4	1	8.3	47	12	1.7
20	41.4	1	8.3	47	17	1.5
21	41.4	1	8.3	47	22	1.3
22	41.4	1	8.3	47	27	1.2
23	41.4	1	8.3	47	32	1.14
24	41.4	1	8.3	47	37	1.04
25	41.4	1	8.3	47	42	1
26	41.4	1	8.3	47	47	0.91
27	41.4	1	8.3	47	52	0.9
28	41.4	1	8.3	47	57	0.85
29	41.4	1	8.3	47	62	0.82
30	41.4	1	8.3	47	67	0.77
31	41.4	1	8.3	47	72	0.75
32	41.4	1	8.3	47	77	0.74
33	41.4	1	8.3	47	85	0.73
34	41.4	1	8.3	47	95	0.73
35	41.4	1	8.3	47	105	0.72

NO	P	IS	pH	PS	t	J
	kPs	M		nm	min	m/s
36	41.4	1	8.3	47	115	0.68
37	41.4	1	10	47	2	2.75
38	41.4	1	10	47	7	2.05
39	41.4	1	10	47	12	1.65
40	41.4	1	10	47	17	1.4
41	41.4	1	10	47	27	1.125
42	41.4	1	10	47	32	1.09
43	41.4	1	10	47	37	1.01
44	41.4	1	10	47	47	0.95
45	41.4	1	10	47	52	0.93
46	41.4	1	10	47	57	0.91
47	41.4	1	10	47	67	0.87
48	41.4	1	10	47	72	0.83
49	41.4	1	10	47	77	0.8
50	41.4	1	10	47	95	0.75
51	41.4	1	10	47	105	0.74
52	41.4	3	6.1	47	2	3.43
53	41.4	3	6.1	47	7	3.13
54	41.4	3	6.1	47	12	2.67
55	41.4	3	6.1	47	17	2.4
56	41.4	3	6.1	47	27	1.98
57	41.4	3	6.1	47	32	1.89
58	41.4	3	6.1	47	37	1.75
59	41.4	3	6.1	47	47	1.56
60	41.4	3	6.1	47	52	1.51
61	41.4	3	6.1	47	57	1.5
62	41.4	3	6.1	47	67	1.43
63	41.4	3	6.1	47	72	1.42
64	41.4	3	6.1	47	77	1.41
65	41.4	3	6.1	47	95	1.34
66	41.4	3	6.1	47	105	1.3
67	41.4	3	8.3	47	0	2.63
68	41.4	3	8.3	47	2	2.55
69	41.4	3	8.3	47	7	2.43
70	41.4	3	8.3	47	12	2.25

Appendix C. (Continued) Experimental Data (Prediction Set)

NO	P	IS	pH	PS	t	J
	kPs	M		nm	min	m/s
71	41.4	3	8.3	47	17	2.2
72	41.4	3	8.3	47	22	1.95
73	41.4	3	8.3	47	27	1.85
74	41.4	3	8.3	47	32	1.75
75	41.4	3	8.3	47	37	1.67
76	41.4	3	8.3	47	42	1.65
77	41.4	3	8.3	47	47	1.55
78	41.4	3	8.3	47	52	1.52
79	41.4	3	8.3	47	57	1.5
80	41.4	3	8.3	47	62	1.49
81	41.4	3	8.3	47	67	1.45
82	41.4	3	8.3	47	72	1.43
83	41.4	3	8.3	47	77	1.4
84	41.4	3	8.3	47	85	1.37
85	41.4	3	8.3	47	95	1.32
86	41.4	3	8.3	47	105	1.27
87	41.4	3	8.3	47	115	1.2
88	41.4	3	10	47	2	2.48
89	41.4	3	10	47	7	2.44
90	41.4	3	10	47	12	2.26
91	41.4	3	10	47	17	2.21
92	41.4	3	10	47	27	1.93
93	41.4	3	10	47	32	1.87
94	41.4	3	10	47	37	1.76
95	41.4	3	10	47	47	1.57
96	41.4	3	10	47	52	1.53
97	41.4	3	10	47	57	1.52
98	41.4	3	10	47	67	1.46
99	41.4	3	10	47	72	1.45
100	41.4	3	10	47	77	1.43
101	41.4	3	10	47	95	1.35
102	41.4	3	10	47	105	1.33
103	41.4	1	10	47	2	2.821
104	41.4	1	10	47	7	2.108
105	41.4	1	10	47	12	1.612

NO	P	IS	pH	PS	t	J
	kPs	M		nm	min	m/s
106	41.4	1	10	47	17	1.457
107	41.4	1	10	47	27	1.178
108	41.4	1	10	47	32	1.116
109	41.4	1	10	47	37	0.992
110	41.4	1	10	47	47	0.93
111	41.4	1	10	47	52	0.899
112	41.4	1	10	47	57	0.884
113	41.4	1	10	47	67	0.853
114	41.4	1	10	47	72	0.837
115	41.4	1	10	47	77	0.806
116	41.4	1	10	47	95	0.76
117	41.4	1	10	47	105	0.744
118	41.4	2	10	47	0	2.8
119	41.4	2	10	47	2	2.632
120	41.4	2	10	47	7	2.296
121	41.4	2	10	47	12	2.016
122	41.4	2	10	47	17	1.848
123	41.4	2	10	47	22	1.652
124	41.4	2	10	47	27	1.568
125	41.4	2	10	47	32	1.456
126	41.4	2	10	47	37	1.372
127	41.4	2	10	47	42	1.316
128	41.4	2	10	47	47	1.232
129	41.4	2	10	47	52	1.176
130	41.4	2	10	47	57	1.148
131	41.4	2	10	47	62	1.12
132	41.4	2	10	47	67	1.092
133	41.4	2	10	47	72	1.078
134	41.4	2	10	47	77	1.064
135	41.4	2	10	47	85	1.036
136	41.4	2	10	47	95	1.008
137	41.4	2	10	47	105	0.98
138	41.4	2	10	47	115	0.924
139	41.4	3	10	47	0	2.6
140	41.4	3	10	47	2	2.561

Appendix C. (Continued) Experimental Data (Prediction Set)

NO	P	IS	pH	PS	t	J
	kPs	M		nm	min	m/s
141	41.4	3	10	47	7	2.522
142	41.4	3	10	47	12	2.34
143	41.4	3	10	47	17	2.184
144	41.4	3	10	47	22	2.054
145	41.4	3	10	47	27	1.989
146	41.4	3	10	47	32	1.82
147	41.4	3	10	47	37	1.768
148	41.4	3	10	47	42	1.742
149	41.4	3	10	47	47	1.664
150	41.4	3	10	47	52	1.586
151	41.4	3	10	47	57	1.573
152	41.4	3	10	47	62	1.534
153	41.4	3	10	47	67	1.482
154	41.4	3	10	47	72	1.469
155	41.4	3	10	47	77	1.43
156	41.4	3	10	47	85	1.404
157	41.4	3	10	47	95	1.352
158	41.4	3	10	47	105	1.326
159	41.4	3	10	47	115	1.3
160	41.4	4	10	47	2	2.574
161	41.4	4	10	47	7	2.543
162	41.4	4	10	47	12	2.444
163	41.4	4	10	47	17	2.366
164	41.4	4	10	47	27	2.236
165	41.4	4	10	47	32	2.106
166	41.4	4	10	47	37	2.002
167	41.4	4	10	47	47	1.872
168	41.4	4	10	47	52	1.846
169	41.4	4	10	47	57	1.794
170	41.4	4	10	47	67	1.742
171	41.4	4	10	47	72	1.69
172	41.4	4	10	47	77	1.664
173	41.4	4	10	47	95	1.586
174	41.4	4	10	47	105	1.555
175	41.4	1	10	110	2	2.635

NO	P	IS	pH	PS	t	J
	kPs	M		nm	min	m/s
176	41.4	1	10	110	7	2.232
177	41.4	1	10	110	12	1.953
178	41.4	1	10	110	17	1.798
179	41.4	1	10	110	27	1.457
180	41.4	1	10	110	32	1.395
181	41.4	1	10	110	37	1.302
182	41.4	1	10	110	47	1.178
183	41.4	1	10	110	52	1.116
184	41.4	1	10	110	57	1.085
185	41.4	1	10	110	67	0.992
186	41.4	1	10	110	72	0.961
187	41.4	1	10	110	77	0.899
188	41.4	1	10	110	95	0.837
189	41.4	1	10	110	105	0.806
190	41.4	2	10	110	0	2.8
191	41.4	2	10	110	2	2.716
192	41.4	2	10	110	7	2.436
193	41.4	2	10	110	12	2.24
194	41.4	2	10	110	17	2.072
195	41.4	2	10	110	22	1.904
196	41.4	2	10	110	27	1.764
197	41.4	2	10	110	32	1.652
198	41.4	2	10	110	37	1.54
199	41.4	2	10	110	42	1.512
200	41.4	2	10	110	47	1.428
201	41.4	2	10	110	52	1.372
202	41.4	2	10	110	57	1.316
203	41.4	2	10	110	62	1.26
204	41.4	2	10	110	67	1.204
205	41.4	2	10	110	72	1.148
206	41.4	2	10	110	77	1.12
207	41.4	2	10	110	85	1.064
208	41.4	2	10	110	95	1.036
209	41.4	2	10	110	105	1.008
210	41.4	2	10	110	115	0.98

Appendix C. (Continued) Experimental Data (Prediction Set)

NO	P	IS	pH	PS	t	J
	kPs	M		nm	min	m/s
211	41.4	3	10	110	0	2.6
212	41.4	3	10	110	2	2.548
213	41.4	3	10	110	7	2.517
214	41.4	3	10	110	12	2.34
215	41.4	3	10	110	17	2.262
216	41.4	3	10	110	22	2.119
217	41.4	3	10	110	27	2.028
218	41.4	3	10	110	32	1.95
219	41.4	3	10	110	37	1.82
220	41.4	3	10	110	42	1.742
221	41.4	3	10	110	47	1.69
222	41.4	3	10	110	52	1.638
223	41.4	3	10	110	57	1.56
224	41.4	3	10	110	62	1.508
225	41.4	3	10	110	67	1.456
226	41.4	3	10	110	72	1.43
227	41.4	3	10	110	77	1.378
228	41.4	3	10	110	85	1.3
229	41.4	3	10	110	95	1.248
230	41.4	3	10	110	105	1.17
231	41.4	3	10	110	115	1.118
232	41.4	4	10	110	2	2.548
233	41.4	4	10	110	7	2.522
234	41.4	4	10	110	12	2.47
235	41.4	4	10	110	17	2.444
236	41.4	4	10	110	27	2.314
237	41.4	4	10	110	32	2.236
238	41.4	4	10	110	37	2.158
239	41.4	4	10	110	47	2.028
240	41.4	4	10	110	52	1.976
241	41.4	4	10	110	57	1.924
242	41.4	4	10	110	67	1.82
243	41.4	4	10	110	72	1.768
244	41.4	4	10	110	77	1.716
245	41.4	4	10	110	95	1.586

NO	P	IS	pH	PS	t	J
	kPs	M		nm	min	m/s
246	41.4	4	10	110	105	1.547
247	41.4	1	10	310	2	3.069
248	41.4	1	10	310	7	3.044
249	41.4	1	10	310	12	2.914
250	41.4	1	10	310	17	2.852
251	41.4	1	10	310	27	2.604
252	41.4	1	10	310	32	2.511
253	41.4	1	10	310	37	2.449
254	41.4	1	10	310	47	2.387
255	41.4	1	10	310	52	2.356
256	41.4	1	10	310	57	2.294
257	41.4	1	10	310	67	2.232
258	41.4	1	10	310	72	2.201
259	41.4	1	10	310	77	2.108
260	41.4	1	10	310	95	2.046
261	41.4	1	10	310	105	1.984
262	41.4	2	10	310	0	2.8
263	41.4	2	10	310	2	2.772
264	41.4	2	10	310	7	2.75
265	41.4	2	10	310	12	2.688
266	41.4	2	10	310	17	2.632
267	41.4	2	10	310	22	2.604
268	41.4	2	10	310	27	2.492
269	41.4	2	10	310	32	2.464
270	41.4	2	10	310	37	2.38
271	41.4	2	10	310	42	2.352
272	41.4	2	10	310	47	2.324
273	41.4	2	10	310	52	2.282
274	41.4	2	10	310	57	2.24
275	41.4	2	10	310	62	2.17
276	41.4	2	10	310	67	2.156
277	41.4	2	10	310	72	2.128
278	41.4	2	10	310	77	2.1
279	41.4	2	10	310	85	2.044
280	41.4	2	10	310	95	2.016

Appendix C. (Continued) Experimental Data (Prediction Set)

NO	P	IS	pH	PS	t	J
	kPs	M		nm	min	m/s
281	41.4	2	10	310	105	1.96
282	41.4	2	10	310	115	1.904
283	41.4	3	10	310	0	2.6
284	41.4	3	10	310	2	2.574
285	41.4	3	10	310	7	2.558
286	41.4	3	10	310	12	2.496
287	41.4	3	10	310	17	2.457
288	41.4	3	10	310	22	2.444
289	41.4	3	10	310	27	2.366
290	41.4	3	10	310	32	2.34
291	41.4	3	10	310	37	2.314
292	41.4	3	10	310	42	2.288
293	41.4	3	10	310	47	2.262
294	41.4	3	10	310	52	2.236
295	41.4	3	10	310	57	2.21
296	41.4	3	10	310	62	2.158
297	41.4	3	10	310	67	2.106
298	41.4	3	10	310	72	2.08
299	41.4	3	10	310	77	2.028
300	41.4	3	10	310	85	2.002
301	41.4	3	10	310	95	1.95
302	41.4	3	10	310	105	1.898
303	41.4	3	10	310	115	1.872
304	41.4	4	10	310	2	2.574
305	41.4	4	10	310	7	2.561
306	41.4	4	10	310	12	2.496
307	41.4	4	10	310	17	2.522
308	41.4	4	10	310	27	2.457
309	41.4	4	10	310	32	2.444
310	41.4	4	10	310	37	2.418
311	41.4	4	10	310	47	2.366
312	41.4	4	10	310	52	2.314
313	41.4	4	10	310	57	2.288
314	41.4	4	10	310	67	2.21
315	41.4	4	10	310	72	2.158

NO	P	IS	pH	PS	t	J
	kPs	M		nm	min	m/s
316	41.4	4	10	310	77	2.106
317	41.4	4	10	310	95	2.028
318	41.4	4	10	310	105	2.002
319	62.1	4	10	47	2	4
320	62.1	4	10	47	7	3.7
321	62.1	4	10	47	12	3.3
322	62.1	4	10	47	17	3.1
323	62.1	4	10	47	27	2.6
324	62.1	4	10	47	32	2.4
325	62.1	4	10	47	37	2.3
326	62.1	4	10	47	47	2.1
327	62.1	4	10	47	52	2.05
328	62.1	4	10	47	57	2
329	62.1	4	10	47	67	1.9
330	62.1	4	10	47	72	1.86
331	62.1	4	10	47	77	1.81
332	62.1	4	10	47	95	1.7
333	62.1	4	10	47	105	1.65
334	41.4	4	10	47	0	2.6
335	41.4	4	10	47	2	2.5
336	41.4	4	10	47	7	2.45
337	41.4	4	10	47	12	2.34
338	41.4	4	10	47	17	2.25
339	41.4	4	10	47	22	2.2
340	41.4	4	10	47	27	2.15
341	41.4	4	10	47	32	2.1
342	41.4	4	10	47	37	2
343	41.4	4	10	47	42	1.98
344	41.4	4	10	47	47	1.92
345	41.4	4	10	47	52	1.9
346	41.4	4	10	47	57	1.87
347	41.4	4	10	47	62	1.83
348	41.4	4	10	47	67	1.78
349	41.4	4	10	47	72	1.72
350	41.4	4	10	47	77	1.64

Appendix C. (Continued) Experimental Data (Prediction Set)

NO	P	IS	pH	PS	t	J
	kPs	M		nm	min	m/s
351	41.4	4	10	47	85	1.6
352	41.4	4	10	47	95	1.57
353	41.4	4	10	47	105	1.54
354	41.4	4	10	47	115	1.53
355	20.7	4	10	47	2	1.42
356	20.7	4	10	47	7	1.39
357	20.7	4	10	47	12	1.37
358	20.7	4	10	47	17	1.36
359	20.7	4	10	47	27	1.34
360	20.7	4	10	47	32	1.33
361	20.7	4	10	47	37	1.32
362	20.7	4	10	47	47	1.3
363	20.7	4	10	47	52	1.29
364	20.7	4	10	47	57	1.28
365	20.7	4	10	47	67	1.26
366	20.7	4	10	47	72	1.25
367	20.7	4	10	47	77	1.24
368	20.7	4	10	47	95	1.22
369	20.7	4	10	47	105	1.21
370	62.1	3	10	47	2	3.98
371	62.1	3	10	47	7	3.4
372	62.1	3	10	47	12	3
373	62.1	3	10	47	17	2.8
374	62.1	3	10	47	27	2.32
375	62.1	3	10	47	32	2.2
376	62.1	3	10	47	37	2.1
377	62.1	3	10	47	47	1.92
378	62.1	3	10	47	52	1.85
379	62.1	3	10	47	57	1.8
380	62.1	3	10	47	67	1.7
381	62.1	3	10	47	72	1.65
382	62.1	3	10	47	77	1.6
383	62.1	3	10	47	95	1.48
384	62.1	3	10	47	105	1.47
385	41.4	3	10	47	0	2.6

NO	P	IS	pH	PS	t	J
	kPs	M		nm	min	m/s
386	41.4	3	10	47	2	2.48
387	41.4	3	10	47	7	2.4
388	41.4	3	10	47	12	2.3
389	41.4	3	10	47	17	2.2
390	41.4	3	10	47	22	2.1
391	41.4	3	10	47	27	2
392	41.4	3	10	47	32	1.93
393	41.4	3	10	47	37	1.87
394	41.4	3	10	47	42	1.81
395	41.4	3	10	47	47	1.75
396	41.4	3	10	47	52	1.66
397	41.4	3	10	47	57	1.58
398	41.4	3	10	47	62	1.53
399	41.4	3	10	47	67	1.5
400	41.4	3	10	47	72	1.48
401	41.4	3	10	47	77	1.45
402	41.4	3	10	47	85	1.4
403	41.4	3	10	47	95	1.34
404	41.4	3	10	47	105	1.3
405	41.4	3	10	47	115	1.28
406	20.7	3	10	47	2	1.34
407	20.7	3	10	47	7	1.33
408	20.7	3	10	47	12	1.32
409	20.7	3	10	47	17	1.3
410	20.7	3	10	47	27	1.27
411	20.7	3	10	47	32	1.26
412	20.7	3	10	47	37	1.25
413	20.7	3	10	47	47	1.23
414	20.7	3	10	47	52	1.22
415	20.7	3	10	47	57	1.2
416	20.7	3	10	47	67	1.18
417	20.7	3	10	47	72	1.17
418	20.7	3	10	47	77	1.16
419	20.7	3	10	47	95	1.14
420	20.7	3	10	47	105	1.13

Appendix C. (Continued) Experimental Data (Prediction Set)

NO	P	IS	pH	PS	t	J
	kPs	M		nm	min	m/s
421	62.1	2	10	47	2	3.75
422	62.1	2	10	47	7	2.9
423	62.1	2	10	47	12	2.5
424	62.1	2	10	47	17	2.2
425	62.1	2	10	47	27	1.8
426	62.1	2	10	47	32	1.68
427	62.1	2	10	47	37	1.58
428	62.1	2	10	47	47	1.43
429	62.1	2	10	47	52	1.38
430	62.1	2	10	47	57	1.3
431	62.1	2	10	47	67	1.22
432	62.1	2	10	47	72	1.2
433	62.1	2	10	47	77	1.16
434	62.1	2	10	47	95	1.08
435	62.1	2	10	47	105	1.06
436	41.4	2	10	47	0	2.8
437	41.4	2	10	47	2	2.5
438	41.4	2	10	47	7	2.2
439	41.4	2	10	47	12	2
440	41.4	2	10	47	17	1.8
441	41.4	2	10	47	22	1.7
442	41.4	2	10	47	27	1.58
443	41.4	2	10	47	32	1.48
444	41.4	2	10	47	37	1.38
445	41.4	2	10	47	42	1.3
446	41.4	2	10	47	47	1.28
447	41.4	2	10	47	52	1.24
448	41.4	2	10	47	57	1.23
449	41.4	2	10	47	62	1.2
450	41.4	2	10	47	67	1.16
451	41.4	2	10	47	72	1.13
452	41.4	2	10	47	77	1.1
453	41.4	2	10	47	85	1.08
454	41.4	2	10	47	95	1
455	41.4	2	10	47	105	0.98

NO	P	IS	pH	PS	t	J
	kPs	M		nm	min	m/s
456	41.4	2	10	47	115	0.95
457	20.7	2	10	47	2	1.38
458	20.7	2	10	47	7	1.25
459	20.7	2	10	47	12	1.18
460	20.7	2	10	47	17	1.14
461	20.7	2	10	47	27	1.05
462	20.7	2	10	47	32	1.01
463	20.7	2	10	47	37	1
464	20.7	2	10	47	47	0.95
465	20.7	2	10	47	52	0.93
466	20.7	2	10	47	57	0.92
467	20.7	2	10	47	67	0.9
468	20.7	2	10	47	72	0.89
469	20.7	2	10	47	77	0.88
470	20.7	2	10	47	95	0.85
471	20.7	2	10	47	105	0.83

APPENDIX D. MATLAB CODE (RBF.M)

```
clear all; close all;
time=cputime;
% read in train and test data
train=load('train.dat'); test=load('test.dat');
% matrix information of two data files
[ra,ca]=size(train);
[rtrain,ctrain]=size(train);
[rb,cb]=size(test);
[rtest,ctest]=size(test);
nboot=100;

% *** simulation preparation*****
ntrain=rtrain;
ntest=rtest;

Ptrain1=train(1:ntrain, 1:ctrain-1)';
Ttrain1=train(1:ntrain,ctrain)';
Ptest1=test(1:ntest, 1:ctest-1)';
Ttest1=test(1:ntest,ctest)';
[n1,n2]=size(Ttest1);

% *** Open A Data File
result=fopen('result.txt','w');

% *** simulation *****
spread=80;
net=newrb(Ptrain1,Ttrain1,1e-5,spread,70,2);
% P    - RxQ matrix of Q input vectors.
% T    - SxQ matrix of Q target class vectors.
% GOAL - Mean squared error goal, default = 0.0.
% SPREAD - Spread of radial basis functions, default = 1.0.
% MN    - Maximum number of neurons, default is Q.
% DF    - Number of neurons to add between displays, default = 25.
%and returns a new radial basis network.

figure(2)
Mtrain=sim(net,Ptrain1);
[trainm,trainc,trainr]=postreg(Ttrain1,Mtrain);
figure(3)
```



```

Mtest= sim(net,Ptest1);
[testm,testb,testr]=postreg(Ttest1,Mtest);
title('Comparison of Predicted and Measured of test data set','FontSize',12,'color','b')
% *** End of Simulation ***

% *** PERFORMANCE EVALUATION ***
% *** Mean Error and Root Mean Square Error of measured and predicted
metest=0.0;rmsetest=0.0;
cum_metest=0.0;cum_rmsetest=0.0;
errtest=(Ttest1-Mtest);
for i=1:ntest
    cum_metest=cum_metest+errtest(i);
    cum_rmsetest=cum_rmsetest+errtest(i)^2;
end
metest=cum_metest/ntest;
rmsetest=sqrt(cum_rmsetest/ntest);
time2=cputime;
time=time2-time;
% *** Print Result Into File ***
fprintf(result,'Computing Time (s)= %6.4f\n',time);
fprintf(result,'Spread          = %6.4f\n',spread);
fprintf(result,'Train set R      = %6.4f\n',trainr);

fprintf(result,'Test set R      = %6.4f\n',testr);
fprintf(result,'Test set ME     = %6.4f\n',metest);
fprintf(result,'Test set RMSE    = %6.4f\n',rmsetest);
fprintf(result,'!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!\n');
fprintf(result,'\n \n');
fprintf(result,'Training Set\n');
fprintf(result,'Time   Measured   NNtrained \n');
for i=1:ntrain
    fprintf(result,'%8.2f %10.5f %10.5f\n',Ptrain1(5,i),Ttrain1(i),Mtrain(i));
end
fprintf(result,'\n \n');
fprintf(result,'*****\n');
fprintf(result,'\n \n');
fprintf(result,'Prediction Set\n');
fprintf(result,'Time   Measured   Predicted \n');
for i=1:ntest
    fprintf(result,'%8.2f %10.5f %10.5f\n',Ptest1(5,i),Ttest1(i),Mtest(i));
end
fprintf(result,'\n \n');
% *** End of Data Output ***
fclose(result);
%=====

```

APPENDIX E. MATLAB CODE (BPNN.M)

```
clear all;

time=cputime;
% read in train and test data
train=load('train.dat');
test=load('test.dat');

% matrix information of two data files
[rtrain, ctrain]=size(train);
[rtest,ctest]=size(test);
% parameters
m2=ctrain-1; m1=ctrain;
m4=400;
m5=25;
m6=1e-10;
nboot=16;
ntrain=rtrain;
ntest=rtest;

% *** simulation*****
Ptrain=train(1:ntrain, 1:ctrain-1)';
Ttrain=train(1:ntrain,ctrain)';
Ptest=test(1:ntest, 1:ctest-1)';
Ttest=test(1:ntest,ctest)';
[n1,n2]=size(Ttest);
T1=zeros(n2,2);
T1(:,1)=Ttest';

% open a file for result
result=fopen('result.txt','w');

% it makes sense to make a loop here to do more than one nn run
prev_testr=0.0;
prev_tme=1.0;
testr=0.0;
tme=1.0;
for nb=1:nboot
    if testr>prev_testr
        prev_testr=testr;
```

```

elseif testr<=prev_testr
    prev_testr=prev_testr;
end
if abs(tme)<prev_tme
    prev_tme=abs(tme);
elseif abs(tme)>=prev_tme
    prev_tme=prev_tme;
end
testr=0.0;

net=newff(minmax(Ptrain),[4,2,1],{'tansig','tansig','purelin'},'trainlm');
% NEWFF(PR,[S1 S2...SN],{TF1 TF2...TFN},BTF,BLF,PF) takes,
% PR - Rx2 matrix of min and max values for R input elements.
% Si - Size of ith layer, for Nl layers.
% TFi - Transfer function of ith layer, default = 'tansig'.
% BTF - Backprop network training function, default = 'trainlm'.
% BLF - Backprop weight/bias learning function, default = 'learngdm'.
% PF - Performance function, default = 'mse'.
% and returns an N layer feed-forward backprop network.

net.trainParam.lr=0.01;
net.trainParam.mc = 0.9;
net.trainParam.min_grad=1e-6;
net.trainParam.show=m5;
net.trainParam.epochs=m4;
net.trainParam.goal=m6;
[net,tr]=train(net,Ptrain,Ttrain);

figure(2)
Mtrain=sim(net,Ptrain);
[trainm,trainc,trainr]=postreg(Ttrain,Mtrain);

figure(3)
Mtest = sim(net,Ptest);
[testm,testb,testr]=postreg(Ttest,Mtest);
title('Comparison of Predicted and Measured of test data set','FontSize',12,'color','b')
fprintf('Run & R= %4.0f %10.4f\n',nb,testr);

%***** PERFORMANCE EVALUATION *****
% *** Mean Error and Root Mean Square Error of measured and predicted

% Mean Error and Root Mean Square Error of measured and predicted
me_test=0.0;rmse_test=0.0;
cum_me_test=0.0;cum_rmse_test=0.0;
err_test=(Ttest-Mtest);
for i=1:ntest

```


APPENDIX F. MATLAB CODE (MULREG.M)

```
clear all; close all;

time=cputime;
% read in train and test data
train=load('train.txt');
test=load('test.txt');

[rtrain, ctrain]=size(train);
[rtest,ctest]=size(test);
% *** simulation*****
ntrain=rtrain;
ntest=rtest;

nsamp=ntrain+ntest;
[nsamp ntest ntrain]

Ptrain1=train(1:ntrain, 1:ctrain-1);
X=[ones(ntrain,1) Ptrain1];
Ttrain1=train(1:ntrain,ctrain);

Ptest1=test(1:ntest, 1:ctest-1);
X1=[ones(ntest,1) Ptest1];
Ttest1=test(1:ntest,ctest);

% result data file
result=fopen('result.txt','w');

% *** multiple regression ***
a1=X\Ttrain1;
Y=X*a1;
Y1=X1*a1;

% *** End of multiple regression ****

% *****PERFORMANCE EVALUATION*****
MaxErr1=max(abs(Y-Ttrain1))
MaxErr2=max(abs(Y1-Ttest1))
r1=corrcoef(Y,Ttrain1);
r2=corrcoef(Y1, Ttest1);
% mse and rmse for training set
```

```

me_train=0.0; rmse_train=0.0;
cum_me_train=0.0; cum_rmse_train=0.0;
errtrain=(Ttrain1-Y);
for i=1:ntrain
    cum_me_train=cum_me_train+errtrain(i);
    cum_rmse_train=cum_rmse_train+errtrain(i)^2;
end

me_train=cum_me_train/ntrain;
rmse_train=sqrt(cum_rmse_train/ntrain)

% mse and rmse for prediction set
me_test=0.0;rmse_test=0.0; cum_me_test=0.0;cum_rmse_test=0.0;
errtest=(Ttest1-Y1);
for i=1:ntest
    cum_me_test=cum_me_test+errtest(i);
    cum_rmse_test=cum_rmse_test+errtest(i)^2;
end
me_test=cum_me_test/ntest;
rmse_test=sqrt(cum_rmse_test/ntest)
time=cputime-time;

% *** Print Result Into File ***
fprintf(result,'Computing Time (s)= %6.4f\n',time);

fprintf(result,'Test set R      = %6.4f\n',r2(1,2));
fprintf(result,'Test set ME      = %6.4f\n',me_test);
fprintf(result,'Test set RMSE     = %6.4f\n',rmse_test);
fprintf(result,'!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!\n');
fprintf(result,'!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!\n');
fprintf(result,'\n \n');
fprintf(result,'Train Set\n');
fprintf(result,' Time   Measured   NNtrained \n');
for i=1:ntrain
    fprintf(result,'%8.2f %10.5f %10.5f \n',Ptrain1(i,5),Ttrain1(i),Y(i));
end
fprintf(result,'\n \n');

fprintf(result,'*****\n')
;

fprintf(result,'*****\n')
;

fprintf(result,'\n \n');
fprintf(result,'Test Set\n');
fprintf(result,' Time   Measured   Predicted \n');

```

```

    for i=1:ntest
        fprintf(result,'%8.2f %10.5f %10.5f\n',Ptest1(i,5),Ttest1(i),Y1(i));
    end
    fprintf(result,'\n \n');

% *** End of Data Output ***
fclose(result);

```

```

plot(Ttest1,Y1,'o','markersize',3)
xlim([0 4]); ylim([0 4]);
line=[0 4];
hold on
plot(line, line,'r')
xlabel('Measured data');
ylabel('Predicted data');
%=====

```

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