MODELING OF ACTIVATED SLUDGE PROCESS BY USING ARTIFICIAL NEURAL NETWORKS

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Approval of the Graduate School of Natural and Applied Sciences

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I certify that this thesis satisfies all the requirements as a thesis for the degree of Master of Science.

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ABSTRACT

MODELING OF ACTIVATED SLUDGE PROCESS BY USING ARTIFICIAL NEURAL NETWORKS

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Current activated sludge models are deterministic in character and are constructed by basing on the fundamental biokinetics. However, calibrating these models are extremely time consuming and laborious. An easy-to-calibrate and user friendly computer model, one of the artificial intelligence techniques, Artificial Neural Networks (ANNs) were used in this study. These models can be used not only directly as a substitute for deterministic models but also can be plugged into the system as error predictors.

Three systems were modeled by using ANN models. Initially, a hypothetical wastewater treatment plant constructed in Simulation of Single-Sludge Processes for Carbon Oxidation, Nitrification & Denitrification (SSSP) program, which is an implementation of Activated Sludge Model No 1 (ASM1), was used as the source of input and output data. The other systems were actual treatment plants, Ankara Central Wastewater Treatment Plant, ACWTP and İskenderun Wastewater Treatment Plant (IskWTP).

A sensitivity analysis was applied for the hypothetical plant for both of the model simulation results obtained by the SSSP program and the developed ANN model. Sensitivity tests carried out by comparing the responses of the two models indicated parallel sensitivities. In hypothetical WWTP modeling, the highest correlation coefficient obtained with ANN model versus SSSP was about 0.980.

By using actual data from IskWTP the best fit obtained by the ANN model yielded R value of 0.795 can be considered very high with such a noisy data. Similarly, ACWTP the R value obtained was 0.688, where accuracy of fit is debatable.

Keywords: activated sludge process, artificial intelligence, artificial neural network, modeling.

ÖZ

AKTİF ÇAMUR PROSESİNİN YAPAY SİNİR AĞLARI KULLANILARAK MODELLENMESİ

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Günümüz aktif çamur modelleri belirleyici karakterlidir ve temel biyokinetiklere dayanarak kurulmuşlardır. Fakat bu modellerin kalibrasyonu fazlasıyla zaman alıcı ve zahmetlidir. Bu çalışmada, aktif çamur işletmelerinin kontrolü için yapay zeka tekniklerinden birisi olan Yapay Sinir Ağları'na (YSA) dayanan kolay kalibre edilebilir ve kullanıcı dostu bir bilgisayar modeli geliştirilmesi denenmiştir. Bu modeler hem direk olarak belirleyici modellerin yerini alabilir hem de hata avcısı olarak belirleyici sistemlere eklenebilirler.

YSA modelleri kullanılarak üç sistemin modellenmesi denenmiştir. Başlangıç olarak, Aktif Çamur Model No 1 (AÇM1) in bir uygulaması olan Tekil Çamur Prosesi Simulasyon (TÇPS) programında kurulmuş hipotetik bir atıksu arıtma tesisi, giriş ve çıkış verilerine kaynak olarak kullanılmıştır. Diğer sistemler, Ankara Merkezi Atıksu Arıtma Tesisi AAT (AMAAT) ve İskenderun AAT (İskAAT), gerçek arıtma işletmeleridir.

TÇPS programındaki hipotetik işletme ve aynı işletmeyi simule eden geliştirilmiş YSA modeline bir sensitivite analizi uygulanmıştır. Sensitivite analizleri parallel

sensitivitiler gösteren iki modelin cevaplarının karşılaştırılmasıyla yapılmıştır. Hipotetik AAT modellenmesinde, YSA modeline karşı TÇPS'den elde edilen en yüksek bağlantı katsayısı yaklaşık 0.980' dir.

İskAAT den gerçek datalar kullanılarak YSA modelinden elde edilen en uygun R değeri 0.795' in böyle hatalı verilerle çok yüksek olduğu düşünülebilir. Benzer olarak, AMAAT' de elde edilen R değeri 0.688 dir ki uyumluluğun doğruluğu tartışılabilir.

Anahtar Kelimeler: Aktif çamur prosesi, yapay zeka, yapay sinir ağları, modelleme.

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LIST OF ABBREVIATIONS

IskWTP	: İskenderun Wastewater Treatment Plant
ACWTP	: Ankara Central Wastewater Treatment Plant
ASP	: Activated Sludge Process
SSSP	: Simulation of Single-Sludge Processes for Carbon Oxidation, Nitrification and Denitrification
Q	: flow rate.
S_s	: Slowly biodegradable solids.
MLVSS	: Mixed Liquor Volatile Suspended Solids
X_{het}	: Heterotrophic Biomass
X_s	: Autotrophic Biomass
ANN	: Artificial Neural Networks
WWTP	: Wastewater Treatment Plant
SRT	: Solid Retention Time
PCA	: Principle Component Analysis
ASM	: Activated Sludge Model
NNTOOL	: Neural Network Toolbox (MATLAB Mathworks Inc.)
HRT	: Hydraulic Retention Time
MR	: Multiple Regression
DBP	: Disinfection by-products
ARX	: Autoregressive Model with External Inputs
RTC	: Real Time Control
FAS	: Fuzzy Adaptive Systems
BNR	: Biological Nutrient Removal
RMSE	: Root Mean Squared Error
TOC	: Total Organic Carbon
IAWPRC	: International Association on Water Pollution Research and Control

PAO : Phosphorus accumulating organisms

bio-P : Biological phosphorus removal

Combo. : Combination

Q_{1inf} : influent flow rate of line 1.

COD_{inf} : influent chemical oxygen demand

Alk. : alkalinity

Q_{ret} : return flow rate

T_{water} : temperature of water

T_{air} : temperature of air

θ_c : solids retention time

eff. : effluent

: number

CHAPTER I

INTRODUCTION

1.1. General

Environmental preservation efforts and developments in the technology have resulted in stringent discharge standards. For this reason, significant amount of investment has gone continuously to wastewater treatment over the years. Consequently the water infrastructures have now been equipped with substantial hardware and software for optimal control and management to compensate for the lack of expertise and staff in the field. Biological treatment systems are usually located away from settlements and the personnel are under constant health threat. Therefore, automation to minimize personnel contact with these systems using expert systems, such as artificial intelligence techniques using neural networks, has become a popular and a very attractive issue.

The new concept about the treatment systems involves *efficient operation* as well as *good design* to reach the goals. It should be understood that only efficiently operated plants can make a maximum out of a good design. Consequently, process control has become an important issue as well as the quality of the design. For the control of the system, some deterministic models, which can also be called as white-box models, have been developed. Although these models give a good insight into the mechanism, they require a lot of hard work before applying to a specific wastewater treatment plant.

The most important of the deterministic models are ASM1, ASM2, ASM3, and ASM2d for activated sludge process (ASP). Determination of the model parameters normally need extensive laboratory and computer work which is often confined to

academic environment. For this reason, particularly for the control of the ASP, a different modeling technique has been attempted in this thesis work.

The new approach involves modeling of ASP using *Artificial Neural Networks* (ANNs). These kinds of models are inspired from the neurological system of humans and try to mimic the human neurological system. Although these models are very far away from the power of its origin, *i.e.* the brain, they showed remarkably good success in the modeling of highly nonlinear systems into which we can also include the ASP.

High quality expertise needed in the process control of wastewater treatment systems made especially automated control, a very attractive subject in the field. But the need for continuous measurement of system variables, which require expert staff, again reduces the efficiency. The ANN models can be a solution to this problem in many aspects. The ANNs need intensive measurement of system variables only for the model development phase. This measurement period is needed for introducing the system to the ANN model being developed. After development of an ANN model of the system is complete, measurements will be done less frequently than before, mainly for cross checking the response of the ANN model with the actual system response. Calibration of ANN models is easier than the white-box models as there are fewer parameters used in the model development process. When the measured variables start showing difference with the response of ANN, the model can be re-trained using the newer data used for cross checking. This process can be automated by embedding the ANN model in an expert system that controls the complete system.

The ANN models are also good error predictors. These models can be used not only on behalf of a deterministic model but also can be plugged into the system as an error predictor. The error prediction can be used for sensor failure detection etc.

In this study, firstly a hypothetical wastewater treatment plant was constructed with the help of an ASM1 model simulator, SSSP program. The SSSP Program was used as a hypothetical treatment plant, and then this hypothetical plant was modeled using ANNs. After development of an ANN model using the SSSP default dynamic input-output pattern, sensitivity analyses were carried out on both models using the same data. Then two actual wastewater treatment plants were modeled. These treatment plants were İskenderun Wastewater Treatment Plant (IskWTP) and Ankara Central Wastewater Treatment Plant (ACWTP). Approximately five months of daily data for IskWTP and one year of daily data for *ACWTP* was used in the modeling processes.

The ultimate aim of this thesis is therefore to develop an ANN model that is capable of predicting outputs from ASP with high fidelity to the actual system; hence somehow model the plant under consideration. To achieve this, various operational parameters will be used as input to predict some of the selected output parameters (influent/effluent chemical oxygen demand etc). In choosing the input parameters, their demonstrated relationships to the output parameters and the biological mechanism were taken into consideration. In addition to that, some combinations of parameters that can be measured on-line continuously will be used to develop the ANN model for precise operation of the system.

CHAPTER II

THEORETICAL BACKGROUND

2.1. Activated Sludge Process

The major biological processes used for wastewater treatment are aerobic, anoxic, anaerobic processes, combined aerobic, anoxic and anaerobic processes and pond processes. The individual processes are further subdivided, depending on whether treatment is accomplished in suspended-growth systems or attached-growth systems or combinations thereof (Tchobanoglous and Burton, 1991).

The activated sludge process, which is an aerobic suspended-growth treatment system, was developed in England by Ardern and Lockett (1914) and was so named because it involved the production of an activated mass of microorganisms capable of stabilizing a waste aerobically. Many versions of the original process are in use today, but fundamentally they are all similar (Tchobanoglous and Burton, 1991).

2.1.1. Process Description

Biological wastewater treatment with the ASP is typically accomplished using a flow diagram as shown in Figure 2.1. Organic waste is introduced into a reactor where an aerobic bacterial culture is maintained in suspension. The reactor contents are referred to as the “mixed liquor”. In the reactor, the bacterial culture carries out the conversion of organic pollutants in accordance with the stoichiometry shown in Equations 2.1 and 2.2 (Tchobanoglous and Burton, 1991).

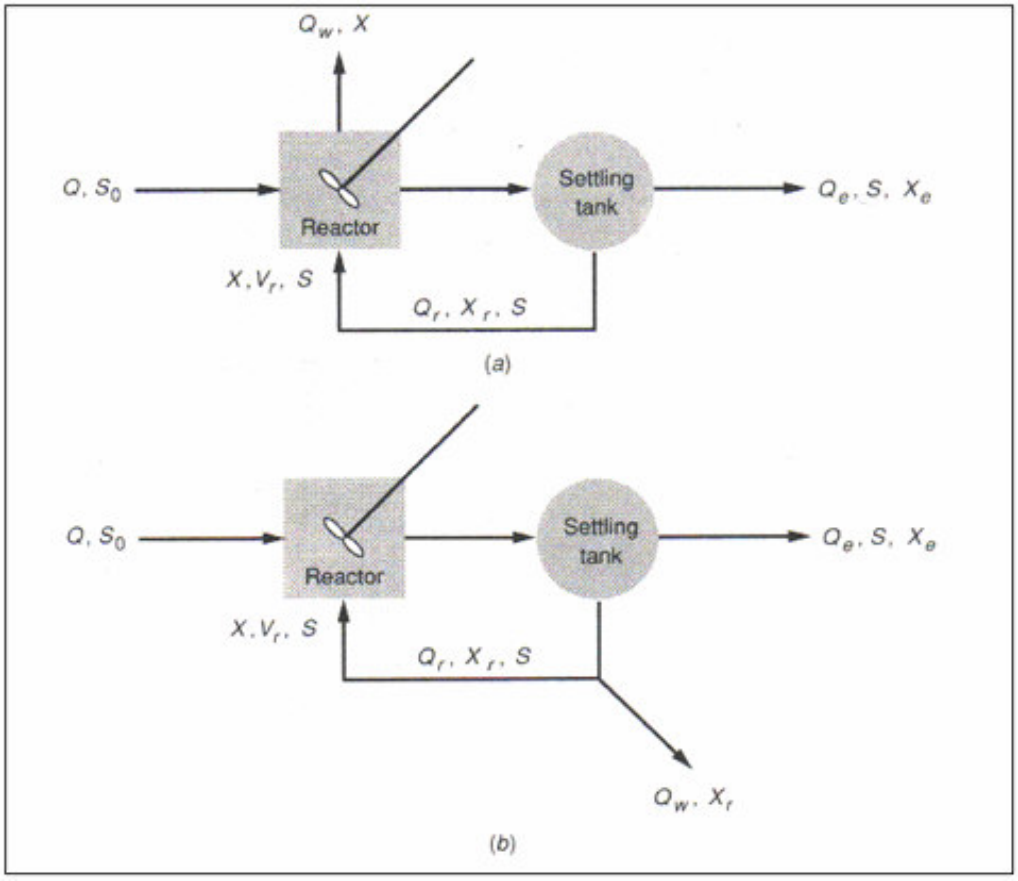


Figure 2.1 Schematic presentation of completely-mixed reactor with biomass recycle and wasting: (a) from the reactor and (b) from the recycle line (Q: flow rate, S: substrate concentration, X: biomass concentration; subscripts r: return, w: waste, 0: influent, e: effluent e.g. Q_r: return flow rate) (Tchobanoglous and Burton, 1991).

Oxidation and synthesis:

$$COHNS + O_2 + nutrients \xrightarrow{bacteria} CO_2 + NH_3 + C_5H_7NO_2 + other\,end\,prod. \quad (2.1)$$

Endogenous respiration:

$$C_5H_7NO_2 + 5O_2 \xrightarrow{bacteria} 5CO_2 + 2H_2O + NH_3 + energy \quad (2.2)$$

COHNS is waste to be treated,

$C_5H_7NO_2$ is the produced new bacterial cells.

The aerobic environment in the reactor is achieved by the use of diffused or mechanical aeration, which also serves to maintain the mixed liquor in a completely mixed regime. After a specified period of time, the mixture of old and new cells are passed into a settling tank, where these cells are separated from the treated wastewater. A portion of the settled cells is recycled to the aeration basin to maintain the desired concentration of organisms in the reactor, and a portion is wasted (Figure 2.1). The portion wasted corresponds to the newly grown cells. The level at which the biological mass in the reactor should be kept depends on the desired treatment efficiency and the efficacy of the aeration system (Tchobanoglous and Burton, 1991).

2.1.2. Process analysis

In the system, reactor is mixed completely via diffused or mechanical aeration used for both mixing and air supply. It is assumed that the concentration of the microorganism in the effluent is negligible. As shown in Figure 2.1 (b), the settling tank serves as an integral part of the activated sludge process. Therefore, for further introduction of the mass balance and also for the development of the kinetic model for the activated sludge process the following assumptions are accepted (Tchobanoglous and Burton, 1991):

- waste stabilization is carried out by the microorganisms occurs in the aerator unit,
- the volume used in the calculation of the mean cell residence time for the system includes only the volume of the aerator unit.

The mean hydraulic retention time, HRT, for the reactor is defined as:

$$HRT = \frac{V_r}{Q} \tag{2.3}$$

where; V_r = volume of the reactor, (L^3)

Q = influent flow rate, (L^3/T)

For the system shown in Figure 2.1(b), the mean cell residence time θ_c is defined as the mass of microorganisms in the reactor over the mass of microorganisms removed plus microorganisms wasted from the system per day, and it is given by:

$$\theta_c = \frac{V_r X}{Q_w X_r + Q_e X_e} \tag{2.4}$$

where;

Q_w = flow rate of liquid containing the biological solids to be wasted from the system, (L^3/T),

Q_e = flow rate of the effluent, (L^3/T),

X_e = effluent microorganism concentration, (M/L^3).

X_r = microorganism concentration in return line, (M/L^3).

The mass balance for the biomass in the entire system represented in Figure 2.1(b) can be written as follows (Tchobanoglous and Burton, 1991):

$$\frac{dX}{dt} V_r = QX_0 - (Q_w X + Q_e X_e) + V_r (r_g') \tag{2.5}$$

where r_g' is the net growth rate of microorganisms within the system.

Assuming that cell concentration in the effluent is zero and steady state condition prevails *i.e.* dX/dt=0 and rearranging Eq. 2.5 gives:

$$\frac{1}{\theta_c} = Yq - k_d \tag{2.6}$$

where; Y = yield coefficient, (M/M),

q = specific substrate utilization rate, (1/T),

k_d = decay coefficient, (1/T).

The mass balance around activated sludge process configuration shown in Figure 2.1(b) regarding substrate can be written as follows (Tchobanoglous and Burton, 1991):

$$\frac{dS}{dt}V_r = QS_0 - QS + V_r(r_s^{'}) \qquad (2.7)$$

2.2. Deterministic Models (ASM1, ASM2, ASM2d, ASM3)

The Activated Sludge Model No. 1 (ASM1; Henze *et al*., 1987) can be considered as the reference model, since it initiated the general acceptance of WWTP models in research and industry. This evolution was undoubtedly supported by the availability of more powerful computers. Even today, the ASM1 model is in many cases still the state of the art for modeling activated sludge systems (Gernaey *et al*., 2004).

ASM1 was primarily developed for municipal activated sludge WWTPs to describe the removal of organic carbon compounds and *N*, with simultaneous consumption of oxygen and nitrate as electron acceptors. The model furthermore aims at yielding a good description of the sludge production. Chemical oxygen demand (COD) was selected as the measure of the concentration of organic matter present. In the model, the wide variety of organic carbon compounds and nitrogenous compounds are subdivided into a limited number of fractions based on biodegradability and solubility considerations (Gernaey *et al*., 2004).

The ASM3 model was also developed for biological *N* removal in WWTPs, with basically the same goals as ASM1. The ASM3 model is intended to become the new standard model, correcting for a number of defects that have appeared during the usage of the ASM1 model (Gujer *et al*., 1999).

Models including biological phosphorus removal (*bio-P*) were first introduced by the ASM2 model (Henze *et al*., 1995), which extends the capabilities of ASM1 to describe *bio-P* removal. Chemical *P* removal via precipitation was also included in

the ASM2. Yet the model does not completely describe the *bio-P* processes (Gernaey *et al*., 2004).

All these models are common in that they need expertise to be calibrated for specific treatment systems that they are tried to be applied. Parameter estimation of the models is very hard in all the deterministic models. In contrast to this, data driven models such as ANN does not need that much expertise. As a result, latter models received attention from the academia as well as the industry.

2.3. Artificial Neural Networks

Hecht-Nielsen defined a neural network as: "… a computing system made up of a number of simple highly interconnected processing elements, which processes information by its dynamic state response to external inputs" (Chitra, 1993).

Neural network technology came from current studies of mammalian brains, particularly the cerebral cortex. Neural networks mimic the way that a human brain copes with incomplete and confusing information set (Chitra, 1993). In general, the human nervous system is a very complex neural network. The brain is the central element of the human nervous system, consisting of nearly 10^{10} biological neurons that are connected to each other through sub-networks.

Each neuron in the brain is composed of a *body*, one *axon* and multitude of *dendrites*. The biological neuron model shown in Figure 2.2 serves as the basis for the artificial neuron. The *dendrites* receive signals from other neurons. The *axon* can be considered as a long tube, which divides into branches terminating in little end bulbs. The small gap between an endbulb and a *dendrite* is called a synapse. The *axon* of a single neuron forms synaptic connections with many other neurons. Depending upon the type of neuron, the number of synapse connections from other neurons may range from a few hundreds to 10^4 (Zilouchian and Jamshidi, 2001).

The ability to learn is a fundamental trait of intelligence. Although a precise definition of learning process is difficult to formulate, *a learning process in ANN context can be viewed as the problem of updating network architecture and connection weights so that a network can efficiently perform a task*. The network usually must learn the connection weights from available training patterns and these patterns should be representative of the system to be modeled (Jane *et al*, 1996).

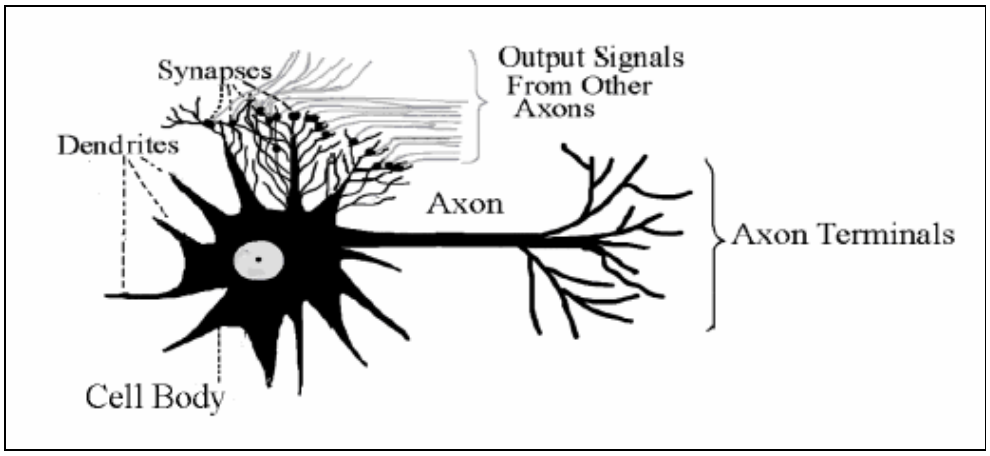


Figure 2.2 A Biological Neuron.

Instead of executing a series of instructions, like an ordinary computer, a neural network responds – ***in parallel*** – to the inputs given to it. The final result consists of an overall state of the network after it has reached a steady-state condition, which correlates patterns between the sets of input data and corresponding output or target values. The final network can be used to predict outcomes from new input data (Chitra, 1993).

Neural networks can learn complex nonlinear relationships even when the input information is noisy and imprecise. Neural networks have made strong advances in the areas of continuous speech recognition, pattern recognition, and classification of noisy data, nonlinear feature detection, market forecasting, and *process control* and *modeling*.

For example, consider how a child *learns* to identify shapes and colors using a toy consisting of different solid shapes (triangles, squares, circles, and so on) and colors that can be inserted into a box only through correspondingly shaped holes and colors. The child learns about shapes and colors by repeatedly trying to fit the solid objects through these holes by trial-and-error attempts. Eventually, the shapes and colors are recognized, and the child is able to match the objects with the holes by visual inspection. Similarly, neural networks learn by repeatedly trying to match the sets of input data to the corresponding output target values. After a sufficient number of learning iterations, the network creates an internal model that can be used to predict for new input conditions (Chitra, 1993).

An *artificial neural network* is an information-processing system that has certain performance characteristics in common with biological neural networks. ANNs have been developed as generalizations of mathematical models of human cognition or neural biology, based on the assumptions that:

1. Information processing occurs at many simple elements called ***neurons***.
2. Signals are passed between neurons over ***connection*** links.
3. Each connection link has an associated ***weight***, which, in a typical neural net, multiplies the signal transmitted.
4. Each neuron applies an ***activation function*** (usually nonlinear) to its net input (sum of weighted input signals) to determine its output signal.

A neural network is characterized by (1) its pattern of connections between the neurons (called its *architecture*), (2) its method of determining the weights on the connections (called its *training* or *learning algorithm*), and (3) its *activation function*.

A neural network consists of a large number of simple processing elements called *neurons* (*units*, *cells*, or *nodes*). Each neuron is connected to other neurons by means

of directed communication links, each with an associated weight. The weights represent information being used by the network to solve a problem.

Each neuron has an internal state, called its *activation* or *activity level,* which is a function of the inputs it has received. Typically, a neuron sends its activation as a signal to several other neurons. It is important to note that a neuron can send only one signal at a time, although that signal is broadcast to several other neurons (Fausett, 1994).

2.3.1. Application Areas of ANNs

The study of neural networks is an extremely interdisciplinary field, both in its development and in its application. The examples of applications of ANNs range from commercial successes to areas of active research that show promise for the future (Jain and Mao, 1996).

In *signal processing*, ANNs were used commercially in suppressing the noise on a telephone line. In *pattern classification*, ANNs are used in character recognition, speech recognition, *EEG* waveform classification, blood cell classification, and printed circuit board inspection. In *optimization*, ANNs are used in a wide variety of fields such as mathematics, statistics, engineering, science, and medicine. In *control*, ANNs are used in *control of dynamic systems* (Jain and Mao, 1996).

2.3.2. Types of ANNs

ANNs are commonly classified by their network topology, node characteristics, learning, or training algorithms (Fausett, 1994). Based on the connection pattern (architecture), ANNs can be grouped into two categories (Figure 2.3- taxonomy of neural network architectures) (Jane *et al*, 1996):

- *Feed-forward networks,* in which network have no looped connections and

- *Feedback* (*recurrent*) *networks,* in which loops occur because of feedback connections.

In the most common family of feed-forward networks, called multilayer perceptron, neurons are organized into layers that have unidirectional connections between them. Different connection patterns yield different network behaviors. Generally speaking, feed-forward networks are *static,* that is, they produce only one set of output values rather than a sequence of values from a given input. Different network architectures require appropriate learning algorithms (Jane *et al*, 1996). A feed-forward network with one hidden layer of neurons is given in Figure 2.3.

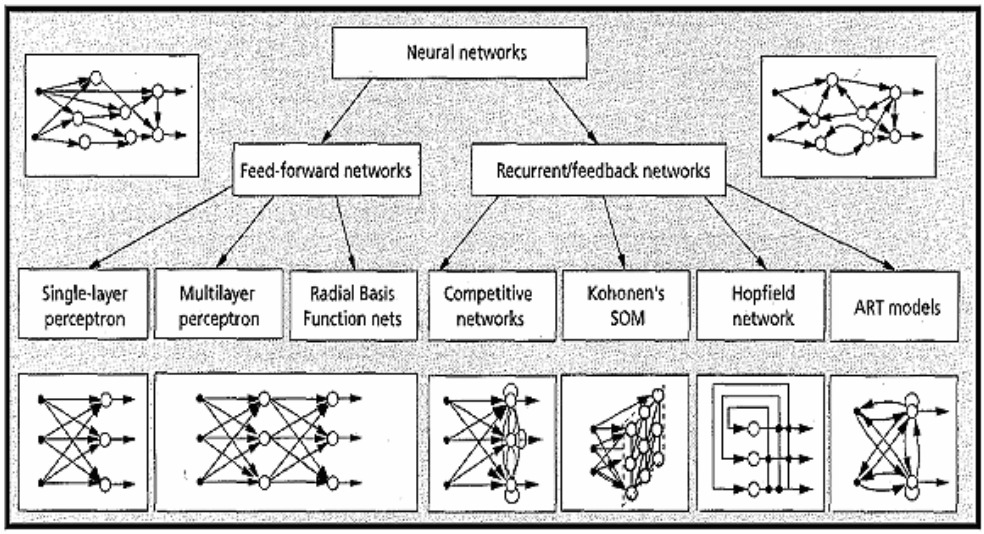


Figure 2.3 Taxonomy of feed-forward and recurrent/feedback neural network architectures.

In a *feed-forward neural network* structure, the only appropriate connections are between the outputs of each layer and the inputs of the next layer. In this topology, the inputs of each neuron are the weighted sum of the outputs from the previous layer. If the weight of a branch is assigned a zero, it is equivalent to no connection between corresponding nodes (Konar, 1999).

For *recurrent/feedback networks*, the inputs of each layer can be affected by the outputs from previous layers (Figure 2.4). In addition, self feedback is allowed. The inputs of the network consist of both external inputs and the network outputs with some delays. Another way of classifying ANNs is mode of training applied. Two modes of training are present in neural net training, *supervised* and *unsupervised learning* networks (Konar, 1999).

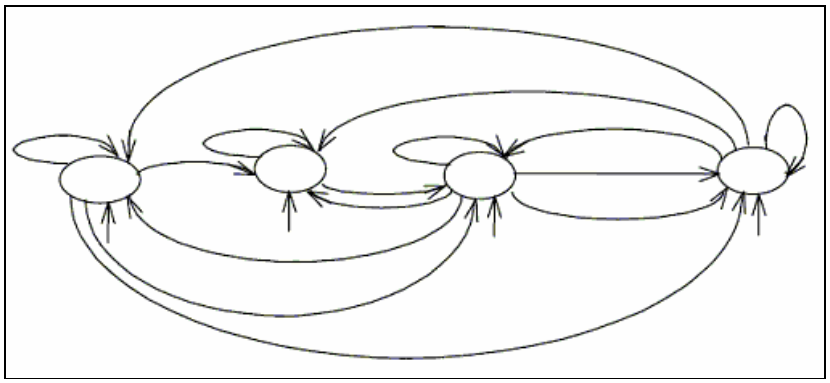


Figure 2.4 An example of a recurrent network with self loops.

Supervised learning requires an external teacher to control the learning and incorporates global information. The teacher may be a training set of data or an observer who grades the performance. Examples of supervised learning algorithms are the least mean square (LMS) algorithm and its generalization, known as the back propagation algorithm, and radial basis function network. In supervised learning, the purpose of a neural network is to change its weights according to the input/output samples (Fausett, 1994).

When there is no external teacher, the system must organize itself by internal criteria and local information designed into the network. *Unsupervised learning* is sometimes referred to as self-organizing learning, *i.e.* learning to classify without being taught. In this category, only the input samples are available and the network

classifies the input patterns into different groups. Kohonen network is an example of unsupervised learning (Konar, 1999).

2.3.3. Typical Feed-forward Backpropagation ANN working

ANN in Figure 2.5 consists of two weight layers corresponding to two neuron layers and connecting three nodal layers; the input layer processes no signal, and this layer is not considered to be a neuron layer. Each node is connected to all the nodes in the adjacent layer, and the signal that is fed at the input layer flows forward layer-by-layer to the output layer. The input layer receives the input vector (data), and one neuron is assigned to each input component (field or variable) (Morshed and Kaluarachchi, 1998).

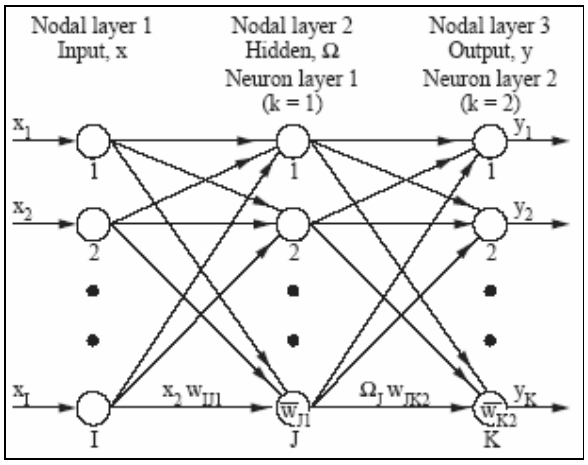


Figure 2.5 Typical backpropagation feed-forward neural network.

The output layer generates the output vector, and one neuron is assigned to each output component. Between these two layers, the hidden layer exists and it has arbitrary number of neurons. Notationally, it shows an *I-J-K* ANN, and the notations used are:

$$x = [x_1, x_2, ..., x_I]^T \tag{2.8}$$

$$\Omega = [\Omega_1, \Omega_2, ..., \Omega_J]^T \tag{2.9}$$

$$y = [y_1, y_2, ..., y_K]^T \tag{2.10}$$

$$\overline{w} = [\overline{w}_1, \overline{w}_2, ..., \overline{w}_{jk}, ..., \overline{w}_{J+K}]^T \tag{2.11}$$

$$w = [w_1, w_2, ..., w_{jk}, ..., w_{J+K}]^T \tag{2.12}$$

where x = input vector of I components; Ω = hidden vector of J components; y = ANN output vector of K components; $\overline{w}$ = threshold weight vector of (J + K) components where $\overline{w}_{JK}$ = threshold of jth neuron in $(k+1)^{th}$ neuron layer; and w = weight vector of J(I + K) components where w_{ijk} is the weight connecting ith neuron in k^{th} neuron layer to j^{th} neuron in $(k+1)^{th}$ layer. ANN may be noted to have $M = (J + K) + J(I + K)$ M weights where M is the total number of weights. *Hecht-Nielsen's* suggestion (1987) is used to define an upper limit of J = (2I + 1) neurons in the hidden layer. Finally, each hidden or output neuron is associated with a transfer function, f(·) (Morshed and Kaluarachchi, 1998).

In simulating the *x*–*y* response for a given *x*, ANN follows two steps. First, *x* is fed at the input layer, and ANN generates Ω as

$$\Omega_j = f\left(\overline{w}_{jk} + \sum_{i=1}^{I} w_{ijk} x_i\right) k = 1 \tag{2.13}$$

Second, ANN presents Ω to the output layer to generate y as

$$y_j = f\left(\overline{w}_{jk} + \sum_{i=1}^{J} w_{ijk} \Omega_i\right) k = 2 \tag{2.14}$$

Equation 2.15 is the ANN response y to x, and y may be expressed as

$$y_j = \Gamma_j(\overline{w}, w, x) \tag{2.15}$$

$$\Gamma(\cdot) = [\Gamma_1(\cdot), \Gamma_2(\cdot), ..., \Gamma_K(\cdot)]^T \tag{2.16}$$

where; $\Gamma(\cdot)$ = underlying x-y response vector approximated by ANN;

$\Gamma_j(\cdot)$ = j^{th} component of $\Gamma(\cdot)$.

Thus, ANN may be viewed to follow the belief that intelligence manifest itself from the communication of a large number of simple processing elements. The transfer

function, f(·), is usually selected to be a nonlinear, smooth, and monotonically increasing function, and two common forms and another common form, the linear transfer functions (purelin() in MATLAB)are :

$$f(x) = sgm(x) = \frac{1}{1+\exp(x)} \tag{2.17}$$

$$f(x) = \tanh(x) = \frac{\exp(x)-\exp(-x)}{\exp(x)+\exp(-x)} \tag{2.18}$$

$$f(x) = purelin(x) = x \tag{2.19}$$

where; sgm(·) is *sigmoid* function,

tanh(·) is hyperbolic tangent function (Morshed and Kaluarachchi, 1998)

purelin(·) is linear function (Matlab Help, 2002).

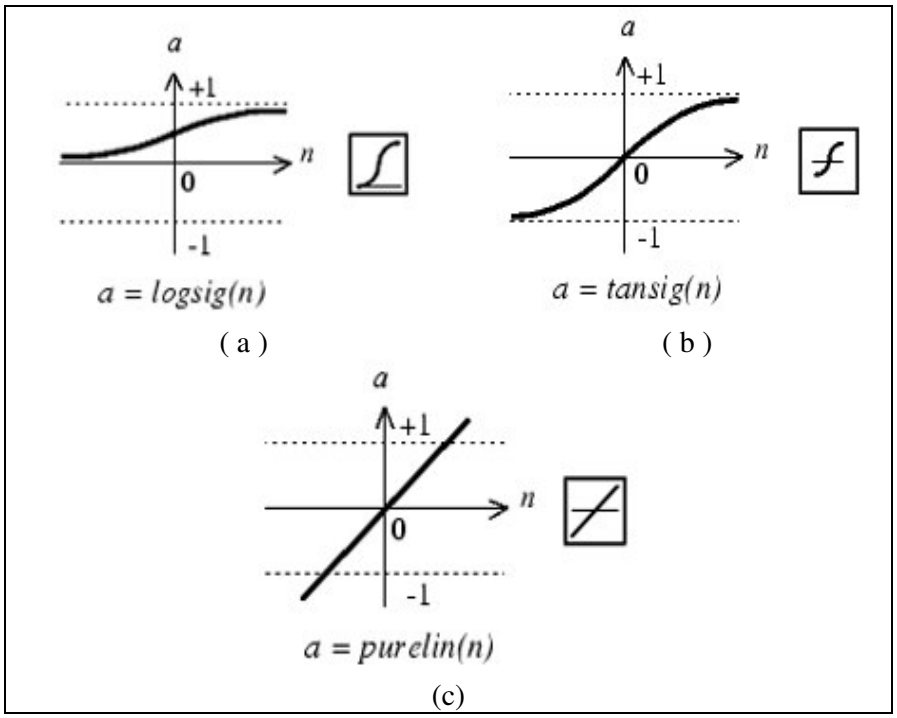


Figure 2.6 Graphs of the typical transfer functions used in ANN models, (a) logarithmic sigmoid function, (b) hyperbolic tangent function,.(c) linear function (Matlab Help, 2002).

2.3.4. Determination of Network Structure

Network structure is defined by the number of hidden layers and number of neurons. These numbers determine the number parameters that must be estimated. This is a very important issue since when the number of parameters to be estimated is insufficient then the model developed may not be able to fit the training data. On the other hand if the number of parameters is too much, this time in relation to available number of training samples, network may loose its ability to generalize (Maier and Dandy, 2001).

Determination of the number of hidden neurons in a hidden layer is generally determined by trial and error. However there exists some upper and lower general bounds to these numbers. Hecht and Nielsen (1987) have suggested the following upper limit for the number of hidden layer neurons in order to ensure that ANNs are able to approximate any continuous function,

$$N^H \leq 2N^I + 1 \tag{2.20}$$

where

N^H : number of neurons in hidden layer,

N^I : number of inputs (number neurons in input layer).

In addition to this formula Roger and Dowla (1994) in order for the network not to over fit the training data, suggested the relationship between the number of training samples (number of input data) and network neuron numbers,

$$N^H \leq \frac{N^{TR}}{(N^I + 1)} \tag{2.21}$$

where

N^{TR} : number of training samples (number of training set data).

2.4. Literature Survey

2.4.1. Uses of Artificial Neural Networks in Ecological Sciences

Most applications of ANNs in biology have been in medicine and molecular biology (Lerner *et al*., 1994; Albiol *et al*., 1995; Faraggi and Simon, 1995; Lo *et al*., 1995). At the beginning of the 90's a few applications of this method were reported in ecological and environmental sciences. For instance, Colasanti (1991) found similarities between ANNs and ecosystems and recommended the utilization of this tool in ecological modeling. In a review by Edwards and Morse (1995) on computer-aided research in biodiversity, important potential of ANNs have been underlined.

Relevant examples are found in very different fields in applied ecology, such as modeling the greenhouse effect (Seginer *et al*., 1994), predicting various parameters in brown trout management (Baran *et al*., 1996; Lek *et al*., 1996a,b), modeling spatial dynamics of fish (Giske *et al*., 1998), predicting phytoplankton production (Scardi, 1996; Recknagel *et al*., 1997), predicting fish diversity (Guégan *et al*., 1998), predicting production: biomass (P:B) ratio of animal populations (Brey *et al*., 1996), predicting farmer risk preferences (Kastens and Featherstone, 1996), etc. Most of these works showed that ANNs performed better than the more classical modeling methods (Lek and Guégan, 1999).

In a study by Lek *et al*. the predictive capacity of multiple regression (MR) versus artificial neural network (ANN) for the estimation of brown trout redds from physical habitat variables in six mountain streams in SW France are compared. Model-predicted and observed values are compared by different statistical parameters, normality and correlation of the residuals. To compare the models (MR and ANN), authors worked with transformed (requirement of MR) and non-transformed (raw data) variables. Three indicators to judge the quality of the results obtained in the MR and ANN are used.

The correlation coefficient R between observed and estimated values, or the determination coefficient R^2; the slope of the regression between values estimated by models and observed values; and the study of residuals $E_i = Y_i - \hat{Y}_i$, their statistical parameters, graphs of normality. The MR model is shown to have difficulty in predicting the low and high values in the data set. Also a negative value prediction is shown by MR model, especially for the low values. For ANN, this problem remains with the transformed values, however with non-transformed variables; an excellent model was obtained capable of restoring values observed over the whole range of the dependent variable. Also ANN model unlike MR model never predicted negative values.

This study showed that MR or ANN can be used to predict the density of brown trout redds from the sampled physical habitat variables, R^2 reached *0.65* in MR and R^2 reached *0.96* in ANN; which gave the better result with the non-transformed variables.

The ANNs constitute a new and alternative approach in ecology. They are able to work with nonlinearly related variables. As a matter of fact they do not set constraints on the variables (e.g. normality and/or nonlinear relationships), better still, they can be more efficient working with raw than with transformed data. Unlike MR, ANN provides simple equations for users but it is possible to easily quantify the contribution of each variable over its range from the weight distribution in the model ANN. It can be concluded that the ANN models can successfully be used in ecological modeling, especially for predictive modeling and ANNs showed better results than the traditionally used models in ecological modeling (Lek *et al.*, 1996).

2.4.2. Uses of ANNs in Environmental Sciences

The ability of two empirical modeling approaches to forecast residual chlorine evolution in two drinking water systems were evaluated (Rodriguez and Sérodes, 1999). The purpose was to compare the forecasting capabilities of a linear model, known as linear autoregressive model, with external inputs (ARX) and a non-linear model (ANNs). The assessment of the benefits in using non-linear models when simulating the decay of residual chlorine in water systems is discussed.

Two case studies were used to compare accuracy of the two kinds of models (ARX vs. ANN). Data from two Quebec (Canada) drinking water systems were used in the study. The first system (denoted as case 1) was a storage tank located within the distribution system of the city of Sainte-Foy. The second system (denoted as case 2) was the main water pipeline of the city of Quebec's distribution system. For both cases, the linear (ARX) and non-linear (ANN) modeling approaches were used to forecast concentrations of residual chlorine at monitored points located downstream from the dose application point (Rodriguez and Sérodes, 1999). Modeling process started from a less complicated structure towards more complicated resulting progressively in higher accuracy.

Another study on water systems was on the real time control of such systems by H. Lobbrecht and Solomatine (2002). Aim of the study was to real time control (RTC) the combined urban and rural water systems. The so-called centralized control requires information from different locations in the water system and hence is sensitive to the communication network breakdown during extreme storm runoff events. To overcome these problems, the application of machine learning methods was proposed, using artificial neural networks and fuzzy adaptive systems (FAS).

The intelligent controllers developed are appeared to be robust and capable of solving RTC problems on the basis of information measured only locally. Computing times were reduced by two orders of magnitude by using local

intelligent controller replicates of central control behavior. This makes the machine-learning techniques (ANN and FAS) useful for application in real-life situations of water management (Lobbrecht and Solomatine, 2002).

A software sensor design based on empirical data obtained from a physical sensor which is responsible for the measurement of ammonia in rivers and wastewater treatment plants was developed by M. H. Masson (1999). The aim of the study was to have a software sensor that was capable of determining the ammonia levels in the field of interest quicker than the physical one that results the measurement in 20 – 25 min. This would allow the control measures to be taken earlier.

In the study of Murtagh *et al*. (2000), a neural network model in the environment and climate Neurosat ("Processing of Environmental Observing Satellite Data with Neural Networks") project was tried for the prediction of oceanic upwelling of the Mauritanian coast, using sea surface temperature (SST) images, and real and model meteorological data for the year of 1982. The overall themes of the study were data and information fusion. The empirical and model-based handling of data was characterized by many uncertainties and numerous missing cases; and the development of data-driven pattern recognition and neural network methods. It was sought whether such methods are an alternative to, or are complementary to, large physical simulation and modeling systems.

Studies on development of neural network based sensor systems for environmental monitoring is done by Keller *et al* (1994). The study is comprised of development of three prototype sensing systems that are composed of sensing elements, data acquisition system, computer, and neural network implemented in software.

The first system employs an array of tin-oxide gas sensors and is used to identify the composition of chemical vapors. The second system employs an array of optical sensors and is used to identify the composition of chemical dyes in liquids. The third system contains a portable gamma-ray spectrometer and is used to identify

radioactive isotopes. The aim is to develop compact, portable systems capable of quickly identifying contaminants in the environment (Keller *et al.*, 1994).

2.4.3. Previous Studies on modeling of Activated Sludge Plant using Artificial Neural Networks

The activated sludge process, comprising a biological reactor and a secondary settler, is widely used as secondary treatment for both municipal and industrial wastewaters. The effective control of such a process depends, in part, on the ability to simulate the dynamics of both the biological reactor and the secondary clarifier. Considerable effort has therefore been devoted to the modeling of the activated sludge process since the early 1970's.

The advent of neural networks opens another door in the field of modeling and control as they can be coupled with mechanistic models to increase the prediction capabilities without necessarily increasing the mathematical complexities in the mechanistic model. The objective of the authors is to report on the improvement of an existing mechanistic model of the activated sludge process using a black box model: ANNs (Côte *et al*., 1995).

A set of 193 hourly samples were used for the modeling of the ANN. The first 140 data were used for the training (learning) process (analogous to the parameter estimation in the mechanistic model), and the remaining data served as a validation file, on which generalizing capability of the network could then be judged.

Coupling of the mechanistic model with the neural network error predictor yielded significant improvement in the simulation of all the variables. This is especially true for the cases where the mathematical expressions of the mechanistic model were insufficient in describing the complex phenomena occurring within the process, e.g. suspended solids in the effluent.

Coupling of neural network error predictor is shown to result in beneficial information about the mechanistic models. If outputs are predicted better by the use of ANNs, which are data driven models, compared to mechanistic models this implies that the mechanistic model can not capture everything underlying in the system. This is a clear indication that the experimental data contains dynamic behavior that has not been encapsulated in the mechanistic model and the ANN modeling effort would lead to a better model (Côte *et al*., 1995).

A virtual software sensor for optimal control of a wastewater treatment process is tried to be developed (Choi and Park, 2001) using artificial neural networks as a modeling tool coupled with principle component analysis (PCA).

The influent wastewater quality data that were measured daily for 113 days at an industrial wastewater treatment plant was used to derive the ANN model (software sensor). Evaluation of the applicability of a hybrid neural network (PCA + ANN), as a software sensor, was compared with four different methods including multivariate regression, principal component regression, neural networks, and hybrid neural networks. The Total Khjeldal Nitrogen (TKN) was selected as the object output parameter that has to be estimated and 11 parameters were used as input variables. In order to increase the sensitivity of the ANN model and enhance the prediction capability, 11 wastewater parameters were reduced to 5 principle components (PCs), which became the principle input parameters of the improved ANN model.

The study confirmed that in modeling of correlated noisy data, the preprocessing using PCA to reduce the number of input variables was effective. Performance criteria used in the study was RMSE (root mean squared error); which is reduced from 66.50 in ANN to 13.82 in ANN + PCA for the test data (Choi and Park, 2001).

It was shown that an industrial treatment plant can be modeled using ANNs. In this study seven neural networks are used to simulate the treatment plant, one network

for each reactor, and another for the prediction of effluent total organic carbon (TOC) based on the conditions for the last reactors. ASP is selected as removal process because of the purified terephtalic acid in the wastewater (Gontarski *et al.*, 2000).

The following variables were used in the training of backpropagation neural networks in the wastewater treatment plant: (a) the inlet wastewater TOC in each reactor; (b) the ratio of influent to recycled sludge flow; (c) concentration of suspended solids (sludge) in the reactors; (d) concentration of dissolved oxygen in the reactors; (e) average sludge residence time; and (f) parameters related to reaction kinetics (Gontarski *et al*, 2000).

In the study two reactor results were given. The sensitivity analysis based on the two reactors showed that the liquid flow rate and pH of the inlet stream were the most important parameters controlling the plant, where all other data were within the range of data supplied in the training process (Gontarski *et al*, 2000). It is concluded that the use of neural networks can establish a better operating condition, which has been defined by variables such as the splitting ratio of the inlet stream for each reactor. Neural networks are seen to represent a possible aid to operations in order to predict disturbances proactively and act to minimize output fluctuations by making the control of the treatment plant more effective (Gontarski *et al*, 2000).

In a recent study for a major wastewater treatment plant with an average flow rate of 1 million m^3/day, past data of the plant were used in building a neural network model of the plant in the Greater Cairo district, Egypt. BOD (Biochemical Oxygen Demand) and SS (Suspended Solids) in the effluent stream were tried to be modeled. The observed values for 10 months were taken from the laboratory of the treatment plant. Two ANN models for each variable were built and these models have shown high efficiency. Although the efficiency was high enough the authors emphasized the importance of the amount and accuracy of the data as follows: if more data were collected, if the data were less noisy, and if additional parameters

were measured (e.g. pH, temperature, etc.), this would have resulted in an improved predictive capability of the network. Nevertheless, the ANN is a tool that is worth consideration in the prediction of WWTPs (Hamed et al, 2004).

Zeng et al have made a study on modeling a paper mill wastewater treatment plant having coagulation as the main mechanism of removal. In the study the authors tried to model the nonlinear relationship between the pollutant removal rates with the chemicals used for the coagulation using a multi-layer back-propagationn neural network. Gradient descent method was used in model training (namely parameter estimation in the deterministic models) and the results obtained have shown an encouraging accuracy that the model could be used in control and reasonable forecasting was achieved (Zeng et al, 2004).

CHAPTER III

MATERIALS AND METHODS

3.1. Artificial Neural Networks

3.1.1. Backpropagation Algorithm

The demonstration of the limitations of the single-layer neural networks was a significant factor in the decline of interest in neural networks in the 1970s. The discovery by several researchers independently and widespread dissemination of an effective general method of training multilayer neural network played a major role in reemergence of neural networks as a tool for solving a wide variety of problems (Kionar, 1999). Standard backpropagation algorithm will be given in this section.

During feed-forward, each input unit (X_i) receives an input signal and broadcasts this signal to the each of the hidden units Z_1, Z_2… Z_p. Each hidden unit then computes its activation and sends its signal (z_j) to each output unit. Each output unit (Y_k) computes its activation (y_k) to form the response of the net for the given input pattern.

During training, each output unit, compares its computed activation y_k with its target value t_k to determine the associated error for that pattern with that unit. Based on this error, the factor δ_k (k= 1, 2… m) is computed. δ_k is used to distribute the error at output unit Y_k back to all units in the previous layer. It is also used (later) to update the weights between the output and the hidden layer. In a similar manner, the factor δ_j, (j=1, 2… p) is computed for each hidden unit Z_j.

After all the δ factors have been determined, the weights for all layers are adjusted simultaneously. The adjustment to the weight w_{jk} (from hidden unit Z_j to output unit Y_k) is based on the factor δ_k and the activation z_j, of the hidden unit Z_j. The adjustment to the weight v_{ij} (from input unit to X_i to hidden unit Z_j) is based on the factor δ_j and the activation x_i of the input unit.

The algorithm can be written as follows:

Step 0: Weight initialization.

(set to small random values)

Step 1: While stopping criteria is false, do Steps 2-9.

Step 2: For each training pair, do Steps 3-8.

Feedforward:

Step 3: Each input unit (X_i, i =1, 2, …., n) receives input signal x_i and broadcasts this signal to all units in the layer above (the hidden units).

Step 4. Each hidden unit (Z_j, j =1, 2, …., p) sums its weighted input signals, $z\_in_j = v_{0j} + \sum_{i=1}^{n} x_i v_{ij}$, applies its activation function to compute its output signal, $z_j = f(z\_in_j)$, and sends this signal to all units in the layer above (output units).

Step 5. Each output unit (Y_k, k =1, 2, …., m) sums its weighted input signals, $y\_in_k = w_{0k} + \sum_{j=1}^{p} z_j w_{jk}$, and applies its activation function to compute its output signal, $y_k = f(y\_in_k)$.

Backpropagation Error:

Step 6: Each output unit (Y_k, k =1, 2, …., m) receives a target pattern corresponding to the input training pattern, computes its error information term, $\delta_k = (t_k - y_k) f'(y\_in_k)$, calculates its weight correction term (used to update w_{jk} later),

$\Delta w_{jk} = \alpha \delta_k z_{j,}$ calculates its bias correction term (used to update w_{0k} later), $\Delta w_{0k} = \alpha \delta_k$, and sends δ_k to units in the layer below.

Step 7: Each hidden unit (Z_j, j =1, 2, …., p) sums its delta inputs (from units in the layer above), $\delta\_in_j = \sum_{i=1}^{m} \delta_k w_{jk}$, multiplies by the derivative of its activation function to calculate its error information term, $\delta_j = \delta\_in_j f'(z\_in_j)$, calculates its weight correction term (used to update v_{ij} later), $\Delta v_{ij} = \alpha \delta_j x_i$, and calculates its bias correction term (used to update v_{0j} later), $\Delta v_{0j} = \alpha \delta_j$.

Update weights and biases:

Step 8: Each output unit (Y_k, k =1, 2, …., m) updates its bias and weights (j=0, …, 9): $w_{jk}(new) = w_{jk}(old) + \Delta w_{jk}$.

Each hidden unit (Z_j, j = 1,… , p) updates its bias and weights (i = 0, …, n): $v_{ij}(new) = v_{ij}(old) + \Delta v_{ij}$.

Step 9: Test stopping condition.

The mathematical basis of backpropagation algorithm is the optimization technique known as *gradient descent*. The gradient of a function (in this case, the function is the error and the variables are the weights of the net) gives the direction in which the function increases more rapidly; the negative of the gradient gives the direction in which the function decreases most rapidly (Fausett, 1994).

3.1.2. ANN Definitions & Concepts

Initialization is required for the weights of the neural network. Selection of initial weights influences whether the net reaches a global (or only a local) minimum of the error and how quickly it converges.

An ***epoch*** is one cycle through the entire set of training vectors or predefined number of points in the training vectors. Many epochs are required for training a backpropagation neural net. A common variation is batch updating, in which weight updates are accumulated over an entire epoch before being applied.

A relationship among the number of training patterns available, *P*, the number of weights to be trained, *W*, and the accuracy of classification expected, *e*, is summarized as: $W/P = e$.

Data representation **(*normalization of data*)** in neural networks is also a very important issue. In many problems, input vectors and output vectors have components in the same range of values. In many neural network applications the data may be given by either a continuous-valued variable or a "*set* or *range*".

The aim of ***training*** a neural net is to have a balance between correct responses to the training patterns and accurate responses to new input patterns. It is equivalent to parameter estimation in traditional deterministic models. It is not always advantageous to continue training until the total squared error reaches a minimum. *Hecht-Nielsen* suggests using two distinct sets of data during training. One of these sets is used for the weight adjustments, and the other one is used at some interval for calculation of the error. If the error in the second test set continues to decrease, training is continued. When the error in the test set (called validation set in MATLAB NNTOOL Toolbox) starts increasing, the net starts memorizing the training patterns. So the training session was stopped (Konar, 1999).

Stopping criteria can be defined as the criteria which result in stopping the training session. Early stopping is important for improving generalization. In this technique the available data is divided into three subsets. The first subset is the ***training set***, which is used for computing the error gradient and updating the network weights

and biases. The second subset is the ***validation set***. The error on the validation set is monitored during the training process. The validation error will normally decrease during the initial phase of training, as does the training set error. However, when the network begins to overfit the data, the error on the validation set will typically begin to rise. When the validation error increases for a specified number of iterations (called ***max fail*** in MATLAB Neural Network Toolbox), the training is stopped, and the weights and biases at the minimum of the validation error are returned (Matlab Help, 2002).

Network structure was defined before as the number of ***hidden neurons*** and ***hidden layers***. The limits on the number of hidden neurons and hidden layers defined by Hecht and Nielsen (1987) and Rogers and Dowla (1994) were taken into consideration in this study. Especially in ANN models with one hidden layer, the upper of these limits were taken and were tried in the script. There were some space and memory requirement problems in the ANN models with two hidden neurons when running the script.

3.2. MATLAB Neural Network Toolbox (NNTOOL) & Scripting

3.2.1. Introduction to NNTOOL and Graphical User Interface

Model development was carried out by using MATLAB Package Program version 6.5 of Mathworks Company. MATLAB is a package program that consists of toolboxes for various areas of engineering. NNTOOL – Neural Network Toolbox is one of the toolboxes in MATLAB that implements ANNs and is used for the modeling process. For an automated search in the solution space a script is written that creates ANNs for a given training function, in a predefined range of hidden layers, in a predefined range of number of neurons in the hidden layers, etc. The details of script are given in the materials and methods section of the thesis.

MATLAB NNTOOL Toolbox is composed of two *graphical user interface* (GUI). Network/Data Manager (Figure 3.2) deals with the communication between MATLAB console and the NNTOOL, and creation and manipulation and addition or subtraction of data or neural networks. Network (Figure 3.3) provides an interface for initialization, training, simulation etc. of ANNs in the Network/Data Manager.

The NNTOOL main GUI is given in Figure 3.2. GUI can be divided into two parts, the data and network representations on top (Inputs, Outputs, Targets, Networks, Errors, Input Delay States, and Layer Delay States). The data to be used can either be exported from MATLAB console or from MATLAB data file (".mat"). Importing, exporting, deleting new data or new network, and creating new network are done with corresponding buttons.

The second part of the GUI deals with network training, initialization etc as mentioned before. This part implements the model building process. From the second part of the main GUI the second GUI (Figure 3.3) that does initialization, simulating, training, and adapting of neural networks that were either created or exported to the main GUI.

The second GUI does everything on the neural network including showing the view of neural network under consideration, training, initialization, simulation, adaptation and showing the weights of the neural net.

NNTOOL was mainly used in this study to derive more accurate results from a pre-developed neural net using the script written for automatic generation of ANN models. NNTOOL is a very user friendly GUI that can be used in creation of small number of models in specific problem domains.

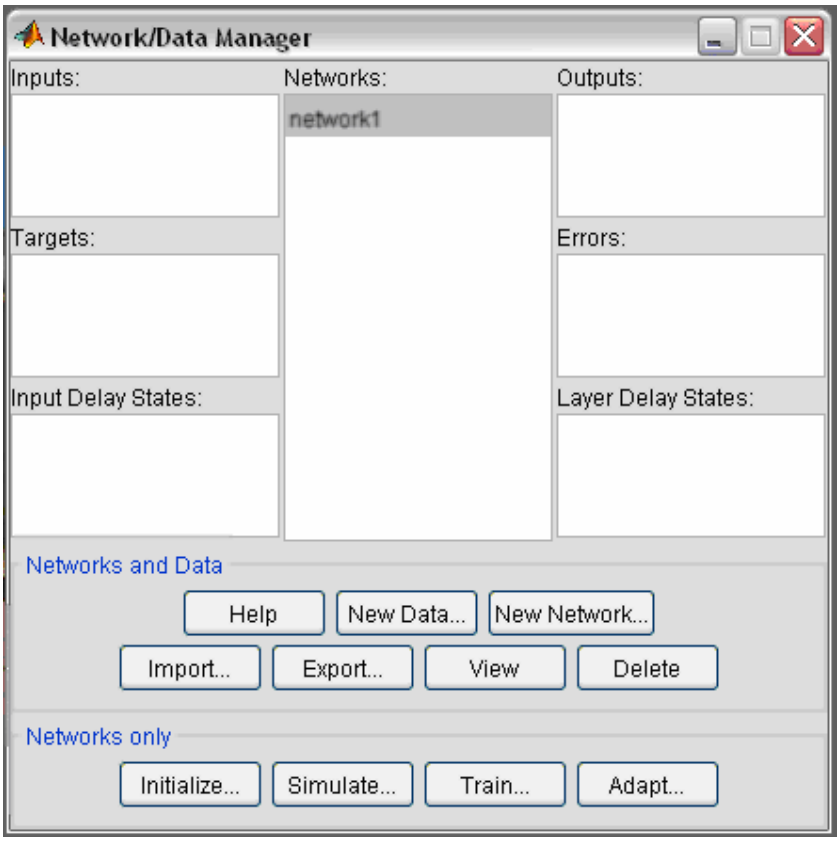


Figure 3.2 Main Graphical User Interface of NNTOOL Toolbox.

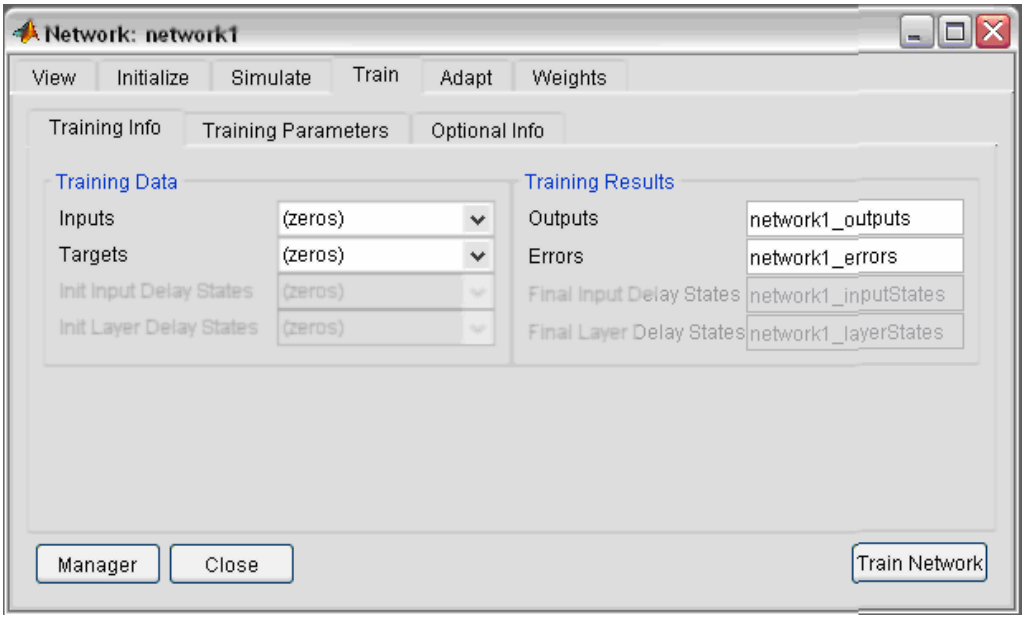


Figure 3.3 Second GUI of NNTOOL Toolbox.

3.2.2. MATLAB Scripting

For the model development, a MATLAB script was written to automatically create ANN models for *IskWTP* and *ACWTP*. The Script does the same thing that NNTOOL GUI does. A graphical user interface (GUI) is shown in Figure 3.3. Script was used to see the change in accuracy when various parameters of created neural nets are changed.

The script has some different versions in which some main structures of the neural nets were changed. For example one version of the script creates only neural nets with only one hidden layer, and this script has three different versions in which transfer functions were changed. The same thing has been applied to the one with two hidden layers. The first version of the script is given in Appendix C.

The script mainly takes a data set from MATLAB workspace and then data is normalized into either [0 1] or [-1 +1] range using "*norm01.m*" script written before for [0 1], built-in *premnmx* function for [-1 +1] range. Then the script divides the data into three subsets that will be used as training, validation and test set. The script enters into a loop that creates neural nets for 13 of the MATLAB's training functions. These training functions are listed in Table 3.3.

For each of these training functions, the script enters into a second loop that changes the number of hidden neurons in a predefined range. Before creating the next network, the script trains the network and simulates the network with the given data and makes a regression analysis of the results obtained at the beginning. After that the next network is created and the same procedure above is applied. Also the script saves the figures of the regression analysis of R (correlation coefficient) values greater than some predefined threshold value, figure of observed versus predicted COD, and figure of time series graph for observed versus predicted values of COD.

Table 3.3[*] training functions used to create ANN models using the script.

training function	Brief Explanation
trainb	Batch training with weight and bias learning rules.
trainbfg	BFGS quasi-Newton backpropagation.
trainbr	Bayesian regularization backpropagation
traincgb	Conjugate gradient backpropagation with Powell-Beale restarts
traincgf	Conjugate gradient backpropagation with Fletcher-Reeves updates
traincgp	Conjugate gradient backpropagation with Polak-Ribiere updates
traingd	Gradient descent backpropagation
traingda	Gradient descent with adaptive learning rate backpropagation
traingdm	Gradient descent with momentum backpropagation
traingdx	Gradient descent with momentum and adaptive learning rate backpropagation
trainlm	Levenberg-Marquardt backpropagation
trainoss	One step secant backpropagation
trainscg	Scaled conjugate gradient backpropagation

3.3. SSSP - Simulation of Single-Sludge Processes for Carbon Oxidation, Nitrification & Denitrification

SSSP is selected because it is a very powerful simulator for the activated sludge process including the nitrification and denitrification. In addition, another reason for the selection of the simulator is that it was used in many successful modeling studies in the literature (Sin, 2000).

The SSSP system is an interactive, user-friendly program for simulating the biological transformations occurring in the activated sludge of a wastewater treatment plant performing simultaneous carbon oxidation, nitrification and denitrification. Process rate expressions that model the biological transformations were developed by a task group formed by IAWPRC. These rate expressions have been incorporated into 12 material balances for the heterotrophic and autotrophic

[*] Interested readers can refer to MATLAB Full Product Family Help R13 for more detailed descriptions of these training algorithms.

biomass, soluble substrate, nitrate nitrogen, and other constituents that the task considered significant in the process analysis of single-sludge wastewater treatment plants. Utilizing numerical techniques, this program determines the solution to these material balances for both constant and time dependent inputs.

The treatment plant is modeled as a chain of up to nine completely mixed reactors. The user specifies the process flow scheme, basin volumes, the flow rate to each reactor, the solids retention time (SRT), the kinetic parameters, the concentrations of all components in the feed streams, and the time dependent pattern of all flow rates and concentrations in those streams. Typical values of the kinetic parameters are provided for simulation when complete kinetic data is unavailable. Interested readers can refer to SSSP User's Manual for the model assumptions, parameters, and equations used. In this study the default dynamic example dataset is modeled. Sensitivity analysis is applied on this dataset and the results obtained are given in section results and discussion.

Dynamic solution menu in SSSP program is used to compute the solution to the mass balance equations for input concentrations and flow rates that vary in magnitude over a 24-hour cycle. To use the routine, variations in input (flow pattern) must be supplied over a 24-hour cycle. SSSP program automatically calculates the average flow rate and flow-weighted average concentrations and uses them to compute the starting point for the numerical integration routine. Then the computer repeats the integration over the 24-hour cycle until the variation in the concentrations of the components is the same from one cycle to the next. In other words, the computer determines the response of a system receiving the same 24-hour input cycle day after day. Therefore, the system's response depends only on the daily variation in loading (Bidstrup and Grady, 1987).

The default dynamic example data set was supplied as input files, and they are generated from *typical settled American domestic wastewater constituent.* This data set is provided on the installation package for exploratory simulations into the

behavior of a system to "*typical*" input variations. The average flow rate on the dynamic flow file is 1000 m^3/d (Bidstrup and Grady, 1987). It was mentioned in the SSSP manual that the set of dynamic data supplied was only for exploratory use. In this study, the data was used only for that purpose. Although this data was not as complex as the real world phenomena, this process was used as a practice in understanding the ANN structure and concepts.

3.3.1. ANN Model development from SSSP Simulator Default Dataset

The default dynamic data set of SSSP was used in the modeling process. In this data set, every parameter is given in a separate file. The input files have two columns, the first column is the time and the second column is the corresponding value of the parameter at that time. The extension of the input files is ".fed" and output file extension for the dynamic output is ".dyn". The default input files of the SSSP program consists of 24 hour hourly data of the system variables used in the calculations.

The SSSP Program has two types of data processing, e.i : "steady state solution" and the "dynamic solution", namely. The dynamic solution in SSSP is supplying 24 hour input data using text file(s) therefore dynamic comes from this supplement. Dynamic solution was used in this study. Three system variables were taken into consideration in the model development process for the ANN model. The three variables used are given in the Appendix A. These system variables are flow rate (Q, m^3/d), particulate products (X_i), autotrophic biomass (X_s, mg/l). The output variables that were predicted by the model were mixed liquor volatile suspended solids (MLVSS), heterotrophic biomass (X_{het}, mg/l), and soluble organics (S_s).

Brief descriptions of the variables used in the modeling process are as follows:

X_{het}: *Heterotrophic biomass*- Represents the biomass which uses readily biodegradable substrate as both source of carbon for synthesis and source of energy

for maintaining life functions. It grows under aerobic and anoxic conditions, but not under anaerobic conditions. Decay results in the conversion of biomass into slowly biodegradable substrate and into particulate products which are not biodegradable. Heterotrophs take up ammonia for cell synthesis under aerobic and anoxic conditions, and convert nitrate nitrogen to gaseous N_2 under anoxic conditions.

X_s: *Autotrophic biomass* – Represents the biomass which uses carbon dioxide as its carbon source for synthesis, and converts ammonia into nitrate for energy. It grows only under aerobic conditions. Decay results in the conversion of biomass into slowly biodegradable substrate and particulate products which are not biodegradable. Autotrophs also take up ammonia nitrogen for cell synthesis during aerobic growth. This biomass includes both Nitrobacteria and Nitrosomonas bacteria which are grouped together for the purposes of simulation.

S_s: *Slowly biodegradable COD* – Represents particulate and high molecular weight organic material which is hydrolyzed extracellularly into readily biodegradable COD. The rate of hydrolysis is lower than the rate of uptake of readily biodegradable substrate.

3.4. Ankara Central Wastewater Treatment Plant

Ankara Central Wastewater Treatment Plant (ACWTP) has been constructed for a capacity of 765000 m^3/d wastewater to be treated by using activated sludge process. The treatment plant was scheduled to serve for a population equivalent of six million by year 2025. It has also been designed to include nitrogen and phosphorus removal units in the future.

The plant employs activated sludge process with anaerobic sludge stabilization. Sewerage system of the city was constructed in phase with the construction of the wastewater treatment plant. When the sewerage system is completed, the 98% of the city wastewater will have been collected to be treated by the plant.

3.4.1. Treatment Plant Layout & Dimensions

At the first stage of ACWTP, there are grid chambers, coarse and fine screens, as the standard preliminary treatment units. These are followed by 10 primary sedimentation tanks each with a diameter of 50 m. Primary sedimentation is followed by 5 rectangular aeration tanks of 35m by 153 m. For the final clarification, 20 secondary sedimentation tanks exist each having a 55 m diameter. A battery of 90 surface aerators supplies air to biological reactions. Effluent COD achieved is less than 30 mg/l for most of the time which is below the discharge standards. General layout of the treatment plant is given in Figure 3.1.

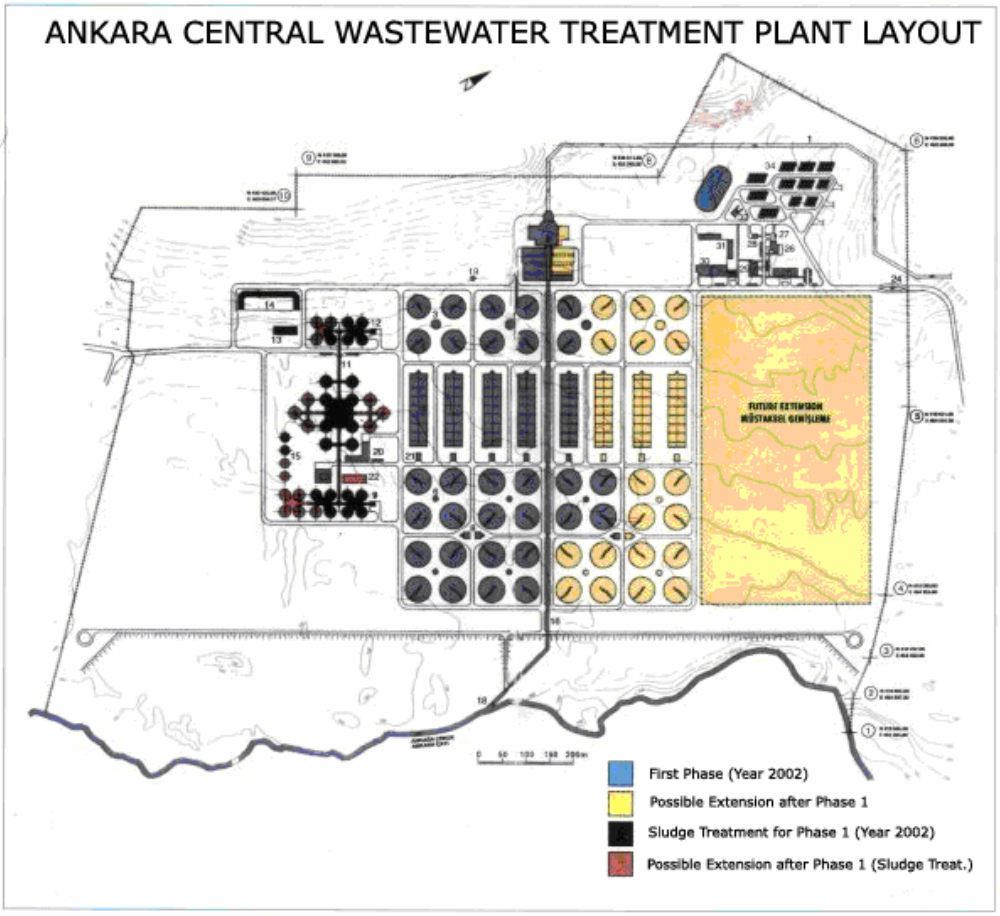


Figure 3.1 General Layout of Ankara Central Wastewater Treatment Plant.

3.4.2. Description of the Data Set

The ACWTP was monitored for five months for the removal of COD. The monitored system variables were ambient air and wastewater temperatures, flow rate, pH, turbidity, alkalinity, suspended solids, COD, and BOD_5 in the influent and effluent wastewater, as well as in different units within the treatment train. Influent wastewater characteristics are given in Table 3.1. The data was obtained from the control engineer of ACWTP. The data obtained included values of variables between May 2002 and February 2003.

Table 3.1 Daily influent wastewater characteristics of ACWTP.

Parameter	Units	Minimum	Maximum	Average	Standard Deviation
Organic Load	%	30	85	66	11
SRT	d	1.46	14.85	3.50	1.51
MLSS	mg/l				
T_{air}	ºC	-14.0	34.0	12.2	9.4
T_{water}	ºC	10.1	21.1	16.0	3.3
Weather State	-	1.0	5.0	1.5	0.8
Q_{Total}	m^3/d	336232	894884	588372	144850
$Q_{1stline}$	m^3/d	164523	377044	269832	45901
pH	-	7.2	7.98	7.52	0.14
Turbidity	NTU	50	225	92	25
Alkalinity	mg/l	250	390	324	23
TSS	mg/l	33	725	189	98
COD	mg/l	136	730	342	90
BOD_5	mg/l	70	380	176	45

Effluent variable to be predicted was COD_{eff}. Effluent COD concentration had a minimum value of 12 mg/l, a maximum value of 80 mg/l, an average value of 43 mg/l, and a standard deviation of 18 mg/l.

3.5. İskenderun Wastewater Treatment Plant

İskenderun Wastewater Treatment Plant is a high technology plant. The plant is a fully automated where process control is administered via SCADA control.

3.5.1. Treatment Plant Layout & Dimensions

İskenderun Wastewater Treatment Plant (*IskWTP*) process train is composed of coarse and fine screens, grid removal, primary sedimentation tanks, activated sludge aeration tanks, and secondary sedimentation tanks. The excess sludge produced in the treatment plant is aerobically digested and dewatered. The design capacity of the treatment plant is 57000 m^3/d, however a capacity of 30000 m^3/d had been used by the end of 2003. The receiving body of the treated water is the Mediterranean Sea.

3.5.2. Description of the Data Set

Two different sets of data belonging to two different time periods were used in this study. The first data set was for March 2002 to December 2002. The second data set was for January 2003 to May 2003. The second data set was used for the model development in this study.

Raw wastewater characteristics of the second data set are given in Table 3.2. There were 33 parameters in the data obtained for the wastewater treatment plant but only 11 were used in model building. This low usage was because either the data were blank or the data was unrelated with the process. The data used for the IskWTP was obtained from the control engineer of the plant.

Table 3.2 Daily influent wastewater characteristics of *IskWTP*.

Parameter	Unit	Minimum	Maximum	Average	Standard Deviation
Q	m^3/d	18,000	42,000	29,85	3,642
pH	-	6.7	8.44	7.82	0.305
Temperature	°C	10.87	27	17.71	3.658
COD mg/L	mg/l	125	330	202	37
TSS mg/L	mg/l	90	208	122	20
BOD	mg/l	71	191	118	33
Sludge Prod.	kg/d	1671	6317	4186	878
SVI	ml/l	69	130	99	12
MLSS	mg/l	2250	2850	2493	118
MLVSS	mg/l	3500	3800	3650	212
θ_c	d	9	-	29	22
COD_{eff}	mg/l	20	67	42	9

CHAPTER IV

RESULTS AND DISCUSSION

In this study, three activated sludge-type treatment plants were modeled by using ANN technique. One of the plants was a hypothetical wastewater treatment plant developed by using SSSP v1.0 simulator (Simulation of Single-Sludge Processes for Carbon Oxidation, Nitrification and Denitrification © 1984 Clemson University). The other two were actual plants operating in Ankara and İskenderun cities in Turkey.

The hypothetical wastewater treatment plant was constructed by using SSSP's default parameters and default dynamic influent wastewater data representing a very simple wastewater treatment plant. The default data was run in SSSP and dependent variable values were obtained for the effluent. The default influent data was based on average wastewater hourly characteristics observed in United States of America. The hourly flow variation in the input file was also based on average USA wastewater with 1000 m^3/d flow rate. Then, a sensitivity analysis was carried out on both SSSP and the constructed ANN model. Both outcomes were then compared to determine the generalization ability of the ANN model.

In the second part of the study, ANN Models for two actual wastewater treatment plants were developed with the data obtained from these plants. A MATLAB Script was written to have an automated search process in the error surface aiming to determine the minimum error on the predictions of the trained model.

4.1. SSSP Model Studies

4.1.1. The SSSP Simulation Program as a Hypothetical Wastewater Treatment Plant

The hypothetical wastewater treatment plant present as default in the SSSP simulation program was used as the first step for the development of an ANN model for the sake of simplicity of data generation, applicability to the model, and for quick output generation.

Another reason for the selection of SSSP simulation program is that, the program uses the acclaimed ASM1 (Activated Sludge Model No 1) model which is currently believed that it accurately describes some of the basic biological mechanisms underlying in the activated sludge process. In addition, using a mechanistic model simulator generates as much data needed for the training of an ANN model. The SSSP model has already been used with success for the modeling of ACWTP Ankara Central Wastewater Treatment Plant) and results have been published in the literature by Sin (Sin, 2000).

The data used in the model development process is given in Table A.1. The output of the SSSP program corresponding to the data set is given in Table A.2. These influent-effluent data pairs were used in the ANN model development for the hypothetical wastewater treatment plant. The input data set used in ANN model building was consisted of variables of Q, X_s, X_i. In response, the ANN model returned effluent variables of MLVSS, S_s, X_{het}.

Input and output variable definitions of the SSSP program were given in Section 3.5.1. The effluent variable data computed by the SSSP program was produced a data set with 30 min intervals, starting at 00:00 hour and ending at 24:00 hours. Thus, the resulting daily data set consisted of 50 data points. However, the number of data was reduced to 24 for use in the ANN modeling by linear interpolation. This

was done by taking average of each two consecutive values. The reason for this was the need to supply the corresponding pairs of inputs and outputs for the ANN model development.

The SSSP Hypothetical Wastewater Treatment Plant was established using the default parameters in the SSSP Program. There are three aeration tanks, each of which has a volume of 200 m^3 and an average daily wastewater flow of 1000 m^3/day fed to the system. The solids retention time (θ_c) is accepted as 10 days. Dissolved oxygen concentration in each tank is assumed to be 4 mg/l. A recycle input of 500 m^3/d is given to the first aeration tank to which all the influent flow is directed.

The graphical output of SSSP using the test input data for the selected variables are given in Figures 4.1, 4.2, and 4.3.

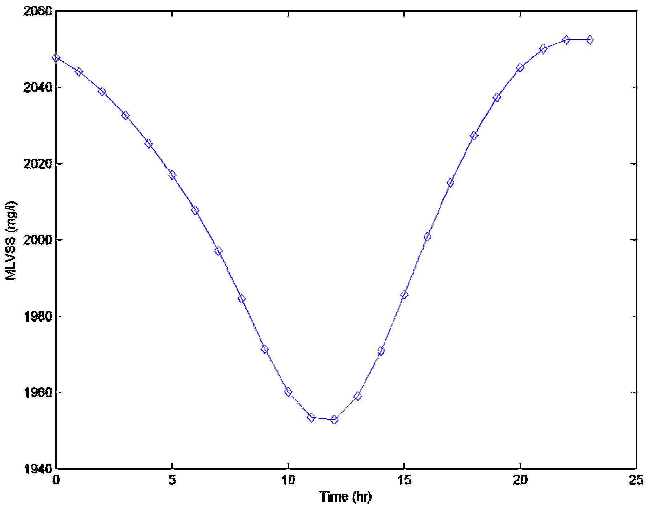


Figure 4.1 MLVSS output of the SSSP simulation.

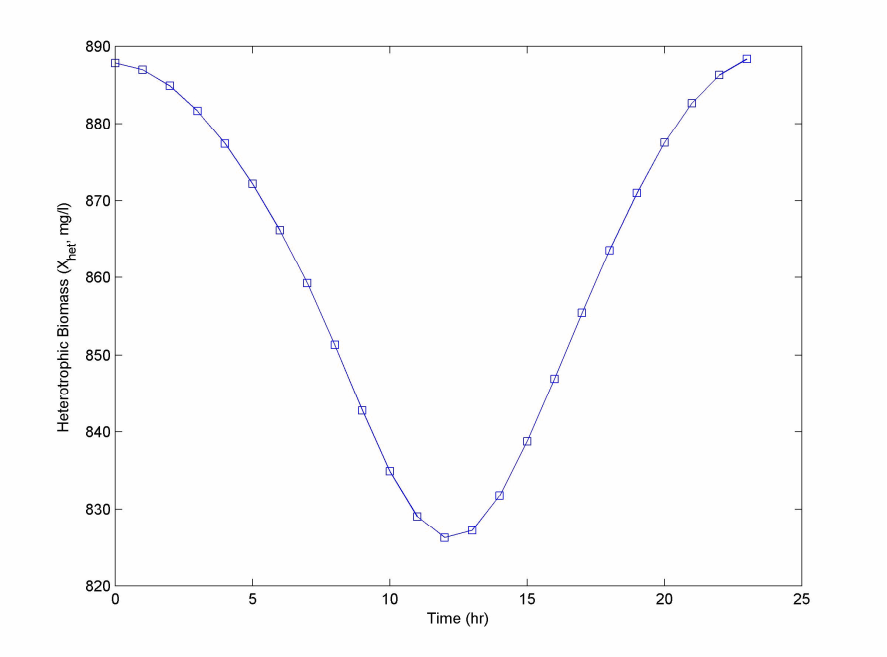


Figure 4.2 X_{het} output of the SSSP simulation.

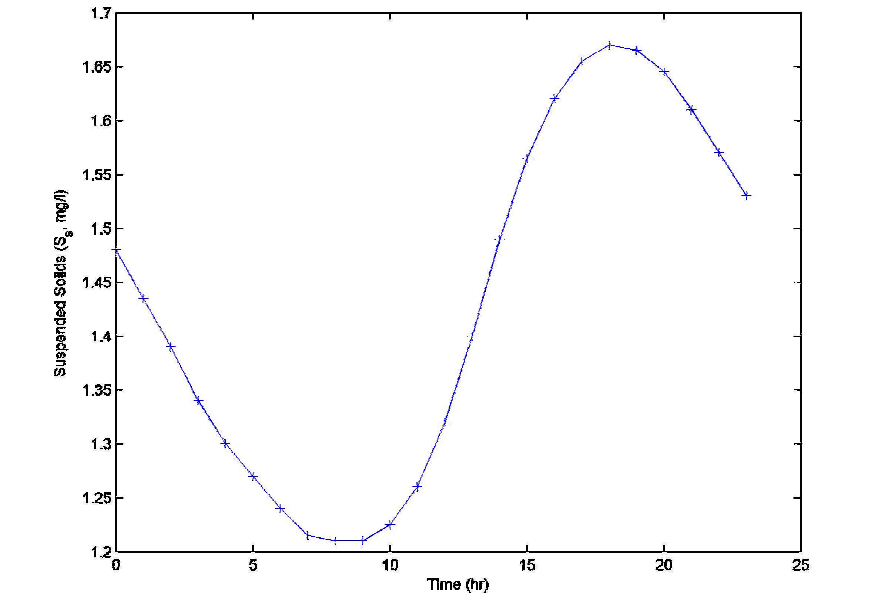


Figure 4.3 S_s output of the SSSP simulation program.

4.1.2. ANN Model Development by SSSP Simulation Program Data

The ANN Model development was tried firstly with one hidden layer manually. The script developed for automatic model generation was used at later stages upon getting familiar with the NNTOOL toolbox GUI. In manual modeling studies, two training functions were tried *(trainb* and *trainbr*). The *trainb* trains the ANN model in *batch mode* which is one of the two modes of weight updating. In this mode of updating, no update occurs until one epoch is completed. That is the ANN model learns slower than the other mode in which updates take effect without waiting for epoch completion. The second training function used was the *trainbr* which updates the assigned weight and bias values according to Levenberg-Marquardt optimization routine. The name of the training function is Bayesian regularization (MATLAB Ref. Manual).

After the script was developed for automatic ANN model generation, this script was used for training. The script was simple and worked as follows: The number of hidden neurons was changed from 2 to 10 for each training function (algorithm). There are 13 training functions supplied by the MATLAB NNTOOL Toolbox for implementing back-propagation algorithm. For every training function, 9 ANN models were developed, having a different number of hidden neurons ranging from 2 to 10, resulting in totally 117 models for each complete run of the script. The ANN models created manually using the NNTOOL GUI were much fewer in number than the models created by using the script. A generic script written is given in Appendix D.

4.1.3. Manual ANN Model Development using NNTOOL GUI

Manual runs showed that the models created with 3 hidden neurons in the hidden layer gave the lowest error and the best fit to the original data. During the manual runs, all the other properties of the ANN model were kept constant. Then, the model with one hidden layer and with 3 hidden neurons was taken as the optimum and

learning rate of the training session was changed. Later, the epoch size was lowered to 6000 as no significant decrease in the mean squared error (MSE) could be observed after this point. Therefore, runs were stopped at 6000 epochs.

The properties of the neural networks used in manual runs are given in Table 4.1. The input layer has three neurons each representing one parameter (Q, X_i, X_s) of the model. The output layer has three neurons each representing a variable to be predicted (MLVSS, X_{het}, S_s).

Table 4.1 Properties of ANN model trials for SSSP runs.

Trial	training Function	Epochs	Goal	Learning Rate	max_fail	Learning Function
Trial1	traingd	6000	0.05	0.070	5	*learngd*
Trial2	traingd	6000	0.05	0.080	5	*learngd*
Trial3	traingd	6000	0.05	0.085	5	*learngd*
Trial4	traingd	6000	0.05	0.090	5	*learngd*
Trial5	trainbr	6000	0.05	0.090	5	*learngd*

The schematic view of the ANN model is given in Figure 4.4. The first layer in the figure is the input layer denoted with the thick black line at the left hand side of the figure. The number "3" below the input layer shows the number of input variables. Then the weight matrix that sends input signals (IW{1, 1}) to the next layer comes. The bias input (b{1}) to the hidden layer is shown with another box below the input weight matrix. The plus sign is an aggregator meaning that incoming signals are added and passed to the next layer. After that, signals are passed to the hidden layer. In the hidden layer box, the type of the transfer function used is given (*tansig* function here). Then again the weight matrix and bias comes, and from these matrices, signals are passed to the next aggregator from where the signals are passed to the output layer having *logsig* as the transfer function.

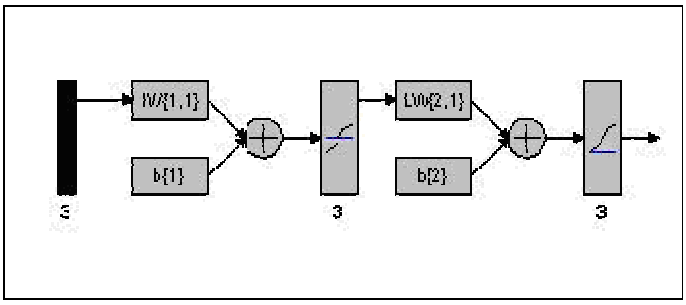


Figure 4.4 Schematic view of ANN Model developed for SSSP.

The differences between the hypothetical WWTP model and actual treatment plant ANN models were: i) In the hypothetical model the model predicts 3 variables whereas in actual wastewater treatment plants only one system variable (effluent COD) was tried to be predicted by the ANN model. ii) In the hypothetical model one hidden layer was used whereas in the real WWTP models there were two hidden layers iii) The training session was increased up to 20000 epochs in the real WWTP models whereas in the hypothetical WWTP model training was stopped at 6000 epochs. These differences evidently resulted from the more complex nature of the biological processes taking effect and the error in the data of the real WWTPs. The choice and implementation of the analysis techniques, quality of technicians, quality of the analytical equipment etc. might have caused the errors in the real WWTPs.

The predictions of the ANN model of MLVSS in the aeration tank for *Trial1* to *Trial5* models are given in Figures 4.5 and 4.6. The best results were obtained with the ANN Model at *Trial5*. The comparison of the SSSP and ANN model outputs for these models is shown in Figure 4.6. Predictions of the last two models, *Trial4* and *Trial5,* had very high correlation with the SSSP data. The R values for these runs were both 0.994, respectively. The improvement obtained towards 4^{th} and 5^{th} trials came from the improving network structure and increase in the learning rate during the training session. Regression plot for *Trial5* is depicted in Figure 4.7. *Trial4* and *Trial5* have given approximately the same result. Therefore distinguishing the response of two trials was very difficult in Figure 4.6

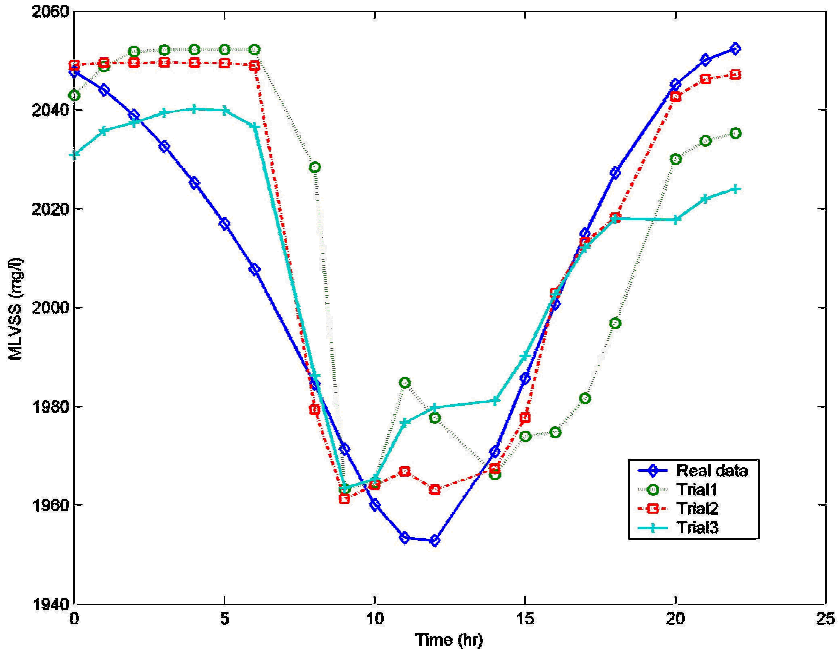


Figure 4.5 The ANN Model run results for MLVSS predictions Trials 1 to 3.

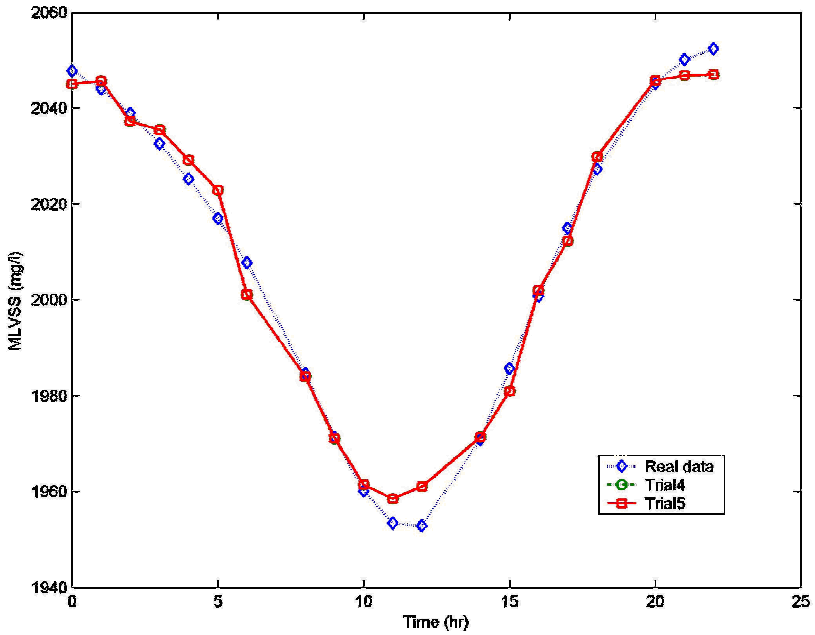


Figure 4.6 ANN Model run results for MLVSS predictions Trials 4 and 5.

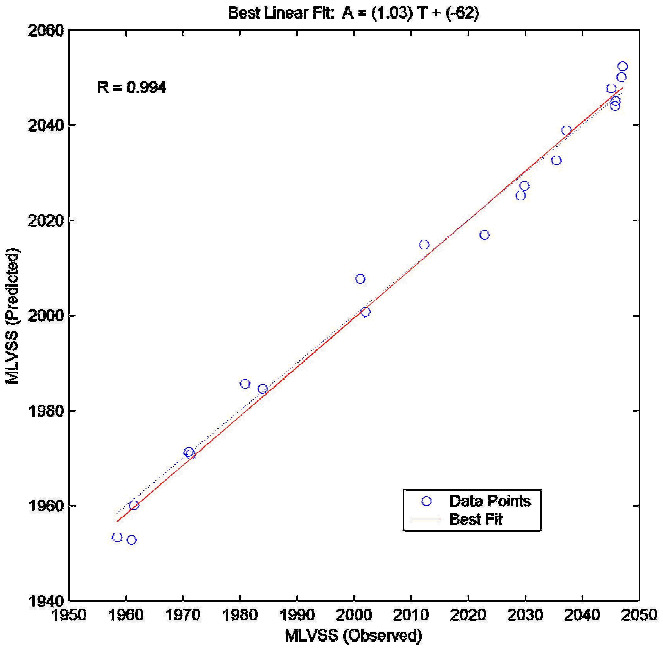


Figure 4.7 Regression analysis result of MLVSS variable for Trial5 ANN model.

The other variables predicted with the same ANN models were the heterotrophic biomass and slowly biodegradable COD in the effluent. The ANN Model *Trial5* gave good fit to the data set generated by SSSP. The second variable, heterotrophic biomass had a very similar pattern with the MLVSS. The prediction capability of the ANN models for the three model variables were very high, implicating extremely good prediction accuracy. The prediction and regression analysis graphs of the other two variables can be found in Appendix B, Figure B.1, B.2, and B.3.

The correlation coefficient between the predicted and real data was *0.994* for MLVSS, which was very high. Evidently such high correlations were due to the synthetic nature of the data, which did not contain the highly complex characteristics of a real plant. The prediction capability of the ANNs was shown with the runs using the SSSP data.

4.1.4. Automated ANN Model Development using a Special Script

The script developed for ANN modeling, which created 117 different models for each run, was used for the data set. Two runs were made using this script. In the first run, data set was divided into 3 subsets. 50% (first 12 hours), 25% (following 6 hours), and 25% (last 6 hours) of the data were allocated for training, 25% validation, and test, respectively. The second run was made with 2 subsets of which 75% (first 18 hours) and 25% (last 6 hours) were utilized for the training and test, respectively. Division into subsets was based on the chronological order of the data. Therefore, the first 12 data points were related with training in both of the runs. The second run was different from the first, such that no validation set was used.

The results obtained from the first run are given in Tables B.1 and B.2. In these tables the results of the models having an R value greater than 0.8 are presented. Therefore, not all of the 117 models are listed. Some of the best fitting models were also selected for sensitivity analyses. The selected models for the first and second runs are given in Table 4.2.

Table 4.2 Selected best ANN models that can be used for sensitivity analyses.

training func.	# of HNs	R_{MLVSS}	R_{Ss}	R_{Xhet}
trainbr (Figure4.8)	3	0.971	0.942	0.938
trainbr	9	0.955	0.969	0.948
traingda	8	0.946	0.992	0.864
trainlm(Figure4.9)	9	0.908	0.989	0.988
trainrp	10	0.920	0.947	0.870

The number of hidden neurons was changed from 2 to 10 for all of the 13 training functions (algorithms) that MATLAB NNTOOL Toolbox provided for both runs. As it can be seen from Table 4.2, Figures 4.8 and 4.9, no further improvement was necessary on the models as high correlation, such as 0.989, indicated perfect match

between the predicted and the observed data. The model developed by using *trainbr* training function (Figure 4.8) consists of 3 HNs in one hidden layer.

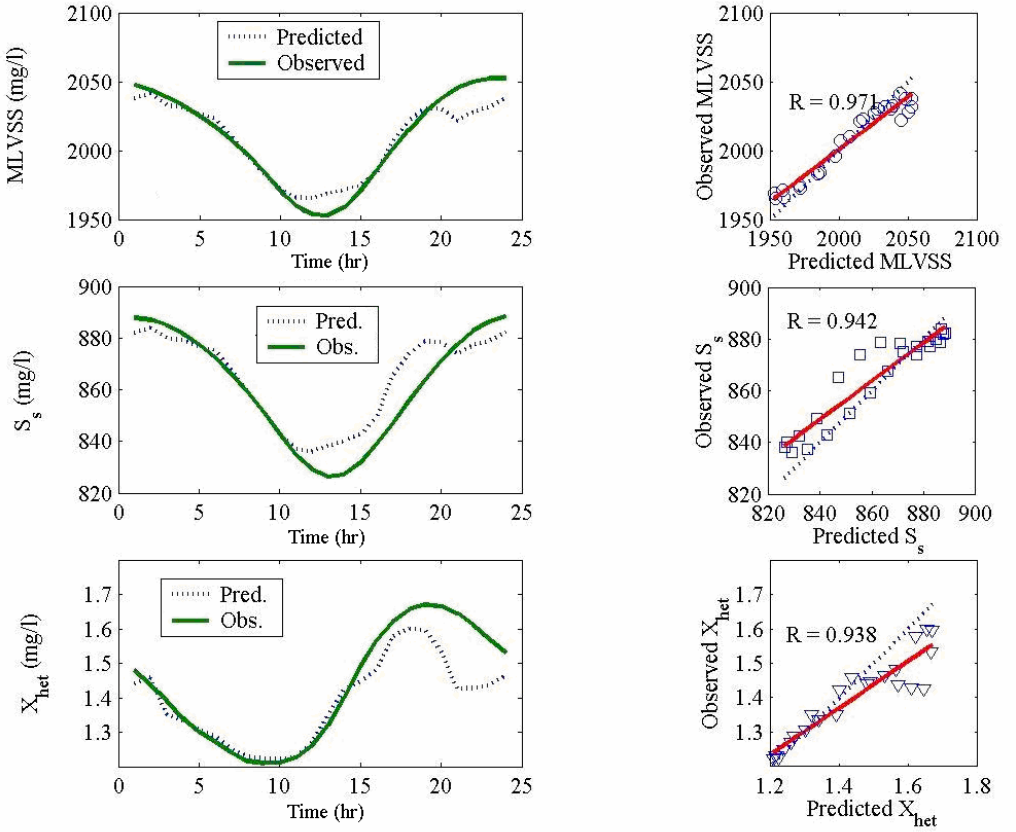


Figure 4.8 Results obtained in ***the 1st run*** with the script: trainbr with number of HNs: 3.

The second successful result was obtained from the *trainlm* (Levenberg-Marquadt backpropagation) algorithm with 9 HNs in one hidden layer (Figure 4.9) and the MSE was 0.0188 while the goal was nil. Again, the results implied no further improvement necessary on the model obtained. Although at this stage of the study further improvements on the models were not necessary, in the actual wastewater treatment plant modeling studies a need for further improving the models became evident.

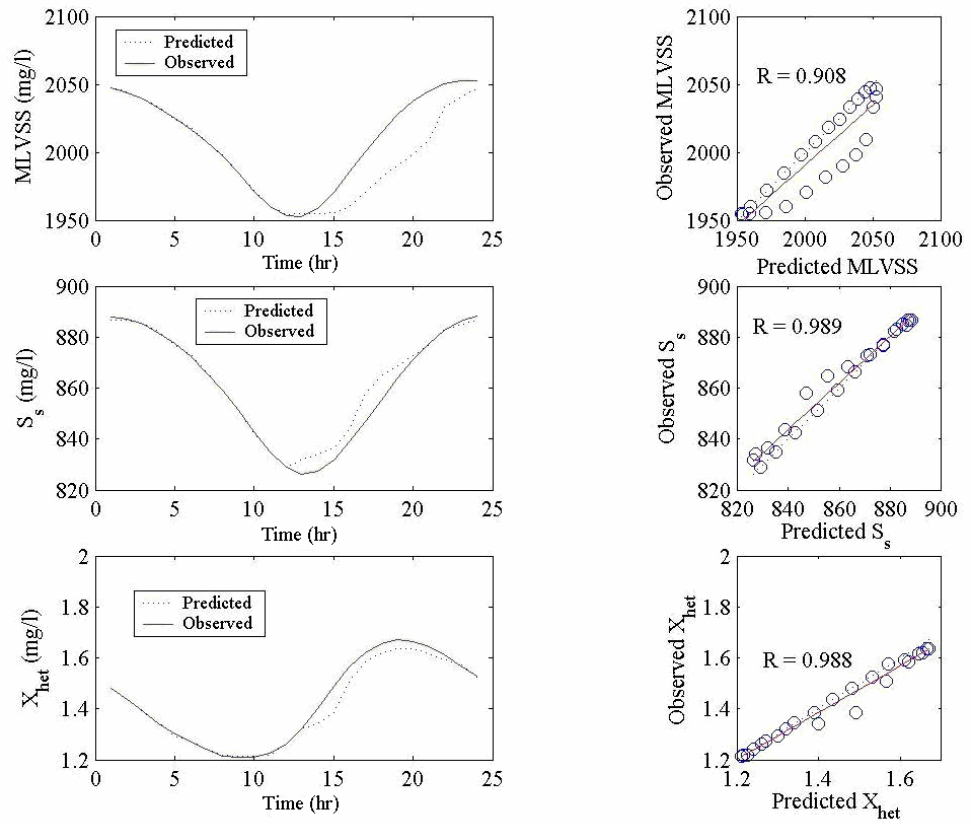


Figure 4.9 Results of ***the 1st run*** with the script: trainlm with number of HN: 9.

In the second run of the script for the SSSP data set, validation set was excluded and the data set was divided into two, *i.e.* 75% of the data (first 18 hours) for training and 25% of which (last 6 hours) for test. The accuracy of the resultant model was higher than the first run which might have been due to the increased amount of data used in this training set.

If the training set includes repeated identical data points then this might result in a poor prediction. Small amount of data which is not able to represent the system may also result in poor model prediction. For these reasons, training sessions might need to be repeated with different training sets constructed from different divisions of the original data set. In the second run the number of training sets was increased from

50% to 75% of the data and the remaining data was used for testing the goodness of fit.

Four of the best models selected are given in Table 4.3. The second model (*traingda with 10 hidden neurons*) was later used in sensitivity analysis. Figures 4.10 and 4.11 show the responses of the ANN models developed using the *traincgp with 4 HNs*, and *traingda with 10 HNs*, respectively.

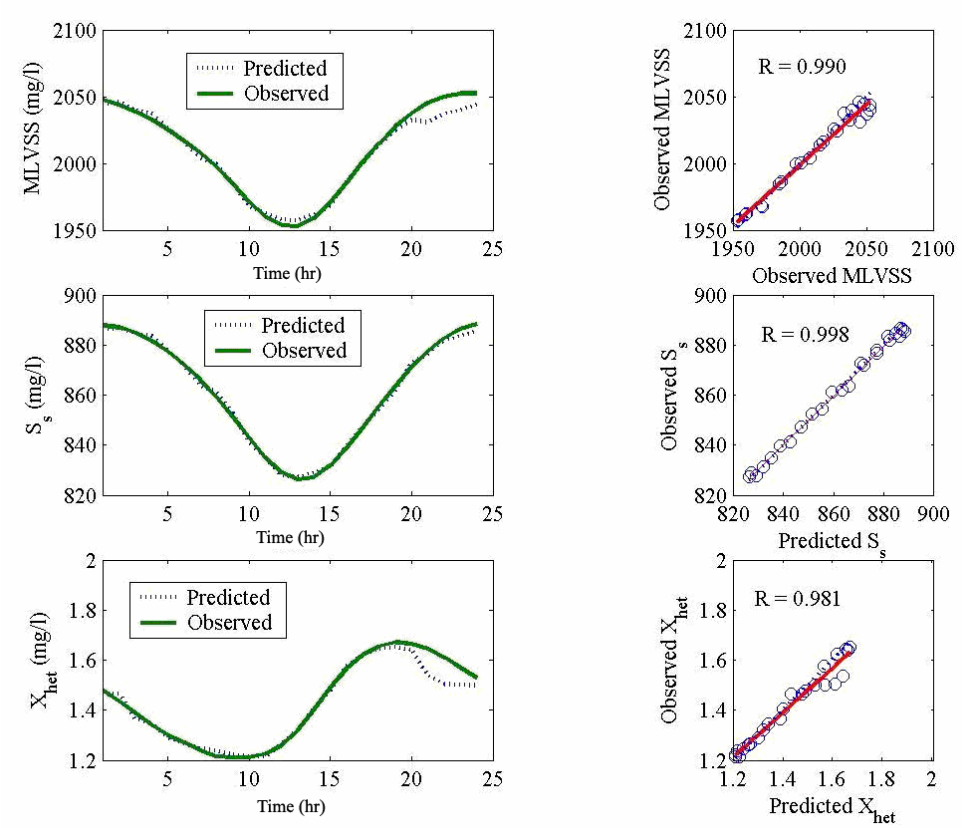


Figure 4.10 The results of ***the 2nd run*** with the script; using *traincgp* with four number of HN

Table 4.3 Results of the second run using the script developed.

training func.	# of HNs	R_{MLVSS}	R_{Ss}	R_{Xhet}
traincgp	*4*	*0.990*	*0.998*	*0.981*
traingda	*10*	*0.998*	*0.993*	*0.992*
traincgp	10	0.997	0.984	0.999
traingdx	6	0.993	0.984	0.999

Although the data was not as complex as the real treatment plant data, the outcome was encouraging as very high correlation results were obtained. This implies that ANNs are able to model the activated sludge process so long as the data supplied adequately represents the particular system.

As described earlier, the validation set was used in the validation of the model and also to check the error incurred during the training session. The validation set is normally different from the training and test sets. Although no validation set was present in the second run, prediction accuracy was higher in this run as compared to the first one with the validation data. This was possibly due to the higher number of training data used in this run.

4.2. Sensitivity Analysis using SSSP Simulation Program

The sensitivity analyses were carried out for all of the three variable inputs, namely Q_{inf}, X_i X_s, used in ANN modeling to see whether the ANN model developed is as sensitive to the system variables as the SSSP model is. The analyses were carried out by changing the values of the original data set by one variable at a time. For example, one of the variables in the data set was decreased by 5%, 10%, and 15%. The sensitivity was tested by comparing the results obtained from SSSP and ANN models with each other. Other variables were kept constant.

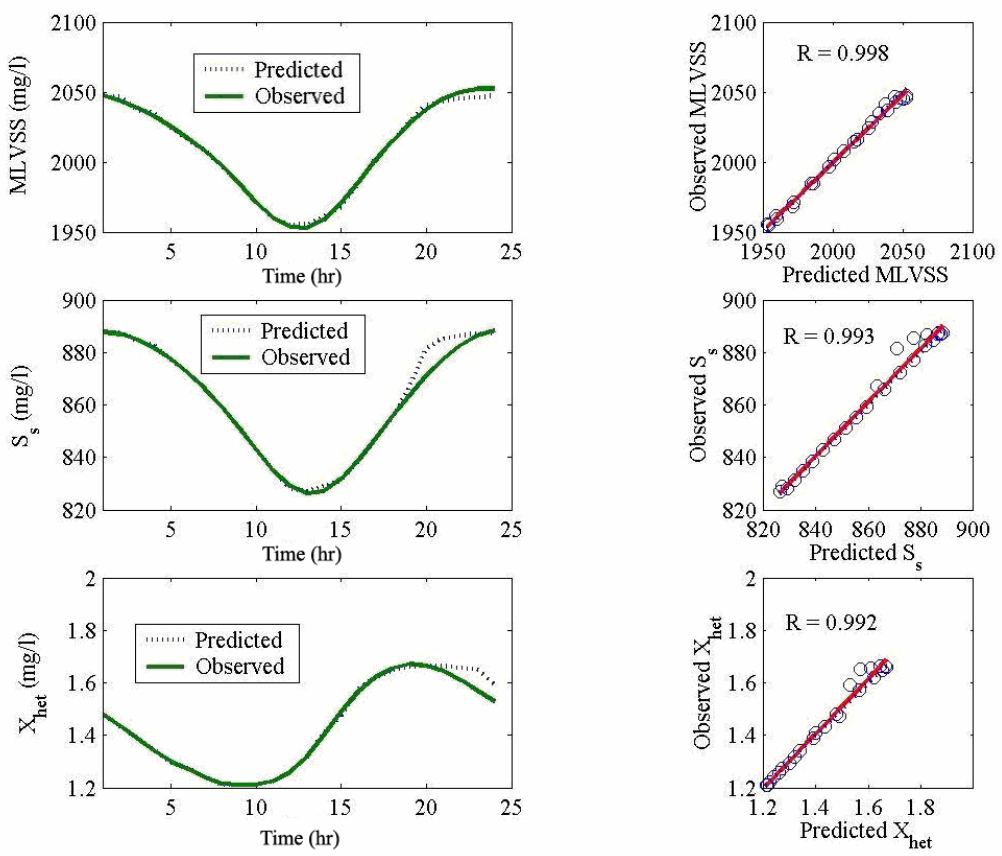


Figure 4.11 The results of ***the 2nd run*** with the script; using *traingda* with ten number of HN

After comprising a data set for a given variable, the best ANN model that was built in the development process (*trainlm*, 10 HNs) was used for prediction. Then the same data set (e.g. 5-15 % decrement in Q_{inf}) was applied to the SSSP Program (representing the hypothetical wastewater treatment plant) to measure the sensitivity of the model to the input variable. After the responses from both of the models were obtained, these were evaluated with reference to the original state. For example, 5% increase in Q_{inf} data produced a set of X_{het} output values, which were then compared with X_{het} output data obtained from the original Q_{inf} values. The output by a (ANN or SSSP) model was compared to the base output. The base output being the output data obtained from the unchanged data.

The changed data was directly applied to the SSSP and after preprocessing (normalization to [0 1] for ANN) for the ANN. However, the ANN model developed was unable to respond to the output values beyond the range of the original data set, as upper and lower boundaries defining the normalization were exceeded. Therefore, to have meaningful analyses, the original data set was normalized with respect to upper and lower limits in the observed data set. This procedure was applied also to the outputs of the system, as ANN model outputs returned a value in the range [0 1] as well. As a result, SSSP response to the original input also set the upper and lower limits for the output normalization. Then, the ANN model was re-trained using this normalized data. The base and preprocessed (new) limits of the data set are given in Table 4.4.

Table 4.4 New minimum and maximum values used in the sensitivity tests.

	Base Minima	New minima	Base Maxima	New Maxima
Q_{inf} (m^3/d)	423	340	1530	1780
X_i (mg/l)	12	9	52	65
S_s (mg/l)	40	30	170	200
MLVSS (mg/l)	1953	1650	2052	2380
X_{het} (mg/l)	826	710	888	1030
X_s (mg/l)	1.21	1.10	1.67	1.80

As given in Table 4.4, MLVSS values in the original SSSP output was varying between 1953 and 2052 and when 5% decrease was applied to Q_{inf} value, SSSP outputs returned 1935 mg/l at the 3rd hour, and this value was outside the range of ANN model ((1935-1953)/(2052-1953), which consequently produced an output less than zero, which was meaningless. To circumvent this problem, the upper and lower limits for both input and output were set beyond the maxima and minima values. However by doing so the ANN models became less sensitive. The maxima and minima values used for normalization are given in Table 4.4.

4.2.1. Sensitivity Tests Based on Flow Rate

The results of all the variables tested with altered Q_{inf} values are given in Figures 4.14 (for X_{het}), 4.16 (for S_s) for the SSSP model; and in Figures 4.13 (for MLVSS), 4.15 (for X_{het}), and 4.17 (for S_s) for the ANN model.

As can be seen from Fig 4.12 and 4.14, sensitivity of the MLVSS and X_{het} variables to Q_{inf}, respectively, is very high in the SSSP model; almost 1:1. In other words, when Q_{inf} was decreased by 15%, MLVSS value also decreased by 15%.

When the ANN model outputs with the varying Q_{inf} were considered, the MLVSS and X_{het} both responded poorly and somewhat in the reverse direction as shown in Figures 4.13 and 4.15, *i.e.* when Q_{inf} was decreased by 15 % both data were nearly converged. This kind of response is contrary to the current understanding of the ASP kinetics. That is, when organic load is reduced, the amount of biomass should also be reduced, as indicated by the SSSP response in Figure 4.12.

As can be seen in Figure 4.16, in the case of S_S, change in Q_{inf} did not affect this parameter at all, within the limits tested. This was not unexpected according to ASP kinetics. Also, in the case of ANN response, as shown in Figure 4.17, change in Q_{inf} had almost no effect on the S_S values. It can be concluded that S_S is not a sensitive parameter after all and ANN results are in accord with this.

4.2.2. Sensitivity Tests Based on Particulate Inert Organic Matter (X_i)

Sensitivity test results indicated that the SSSP model is also very sensitive to X_I with respect to input MLVSS, as indicated in Figure 4.18. The results of these studies are given in Figures 4.18 (for MLVSS), 4.20 (for X_{het}), 4.22 (for S_s) for SSSP model and in Figures 4.19 (for MLVSS), 4.21 (for X_{het}), and 4.23 (for S_s) for ANN model.

It can be concluded that response of ANN to X_i input with respect to MLVSS was somewhat close to that obtained in SSSP, as indicated in Figure 4.18. It can be concluded that the results might improve using dedicated ANN models for each output variables i.e. MLVSS, X_{het}, and S_s. Here, three input variables are entered into the model and three variable outputs are received. In a dedicated model three variables may be entered but one variable output may be obtained. Another reason for the poor prediction of the ANN model could be due to the altered model limits which were changed in the sensitivity data set to avoid minus normalization. This has resulted in the accumulation of the original data set between [0.38 - 0.55] range, which might have resulted in poor training.

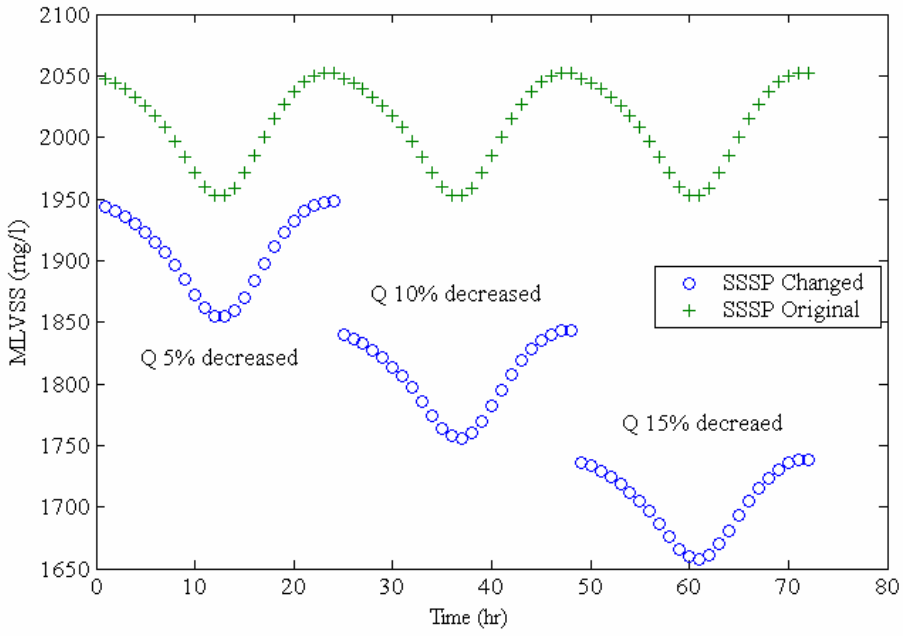


Figure 4.12 Sensitivity test results of MLVSS for SSSP Hypothetical WWTP for changed Q_{inf}.

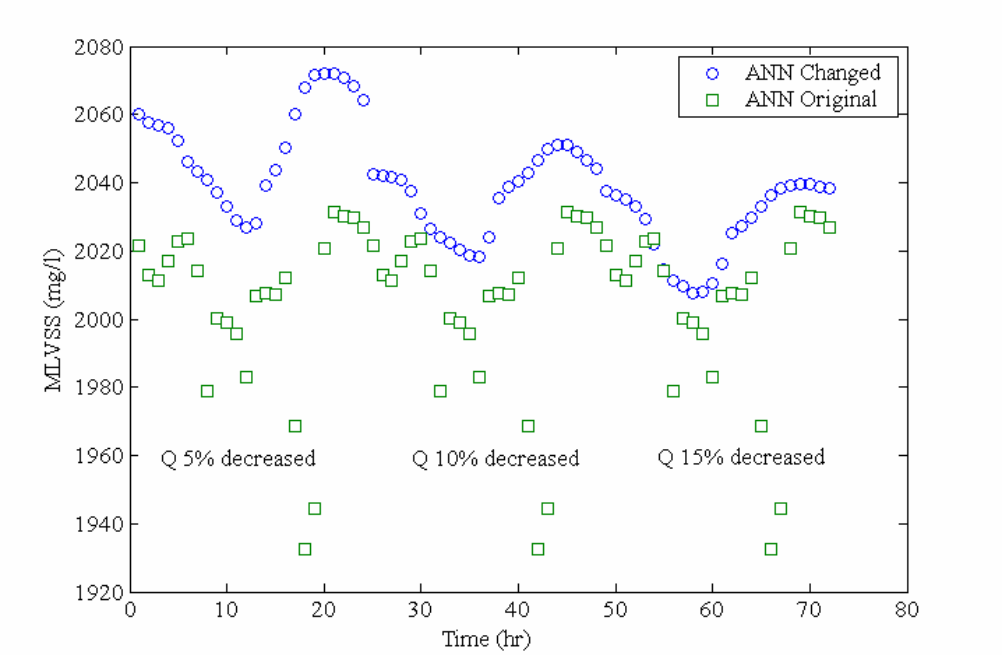


Figure 4.13 Sensitivity results of MLVSS for changed Q_{inf} in ANN Model (*trainlm, 10 HNs*).

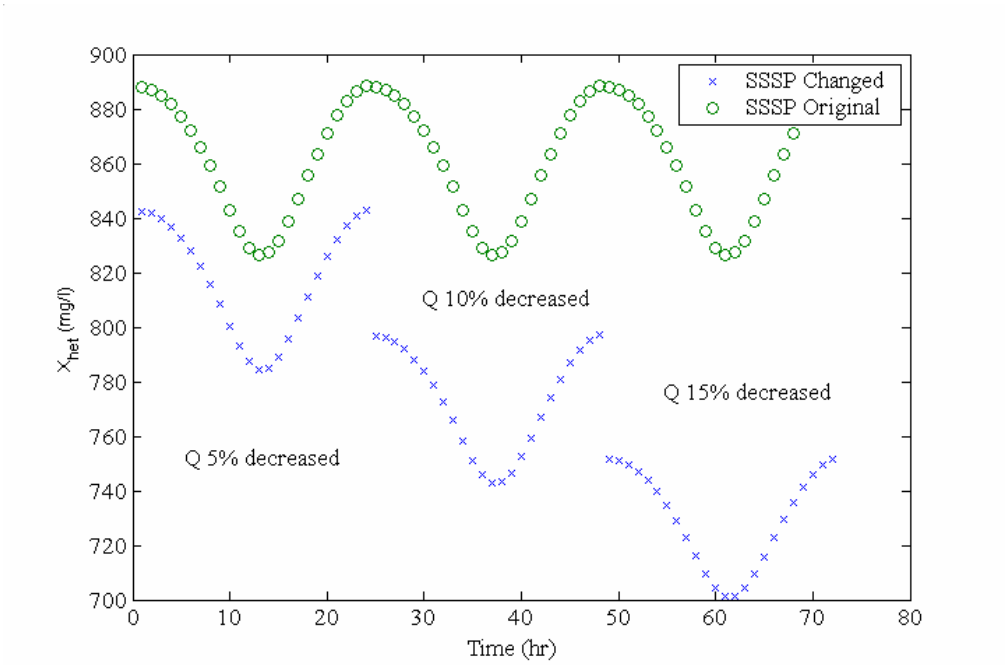


Figure 4.14 Sensitivity results of X_{het} for SSSP Hypothetical WWTP for changed Q_{inf}.

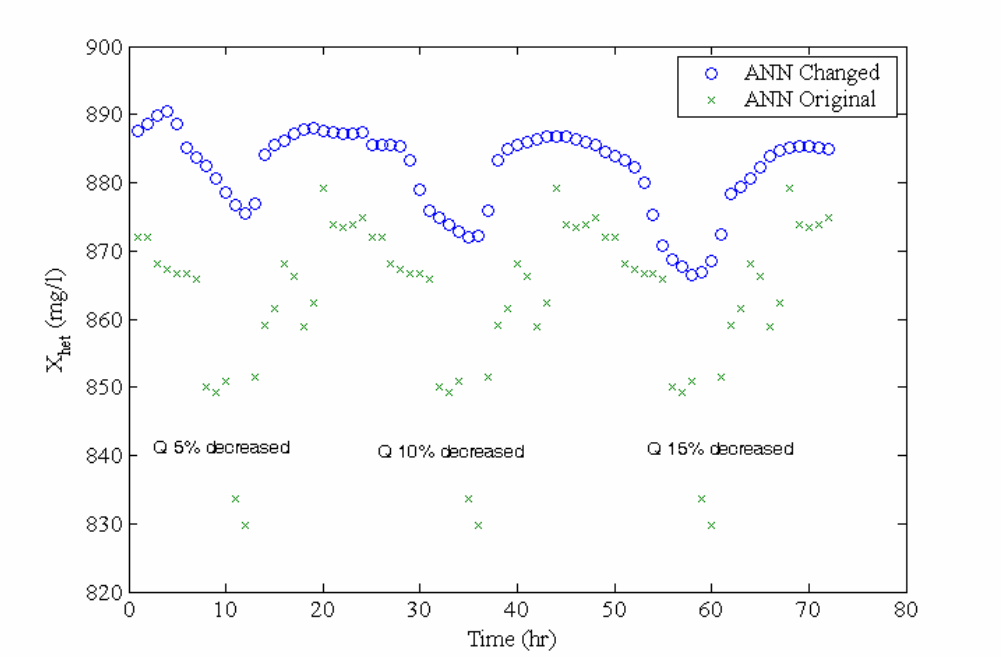


Figure 4.15 Sensitivity results of X_{het} for changed Q_{inf} in ANN Model (*trainlm, 10 HNs*).

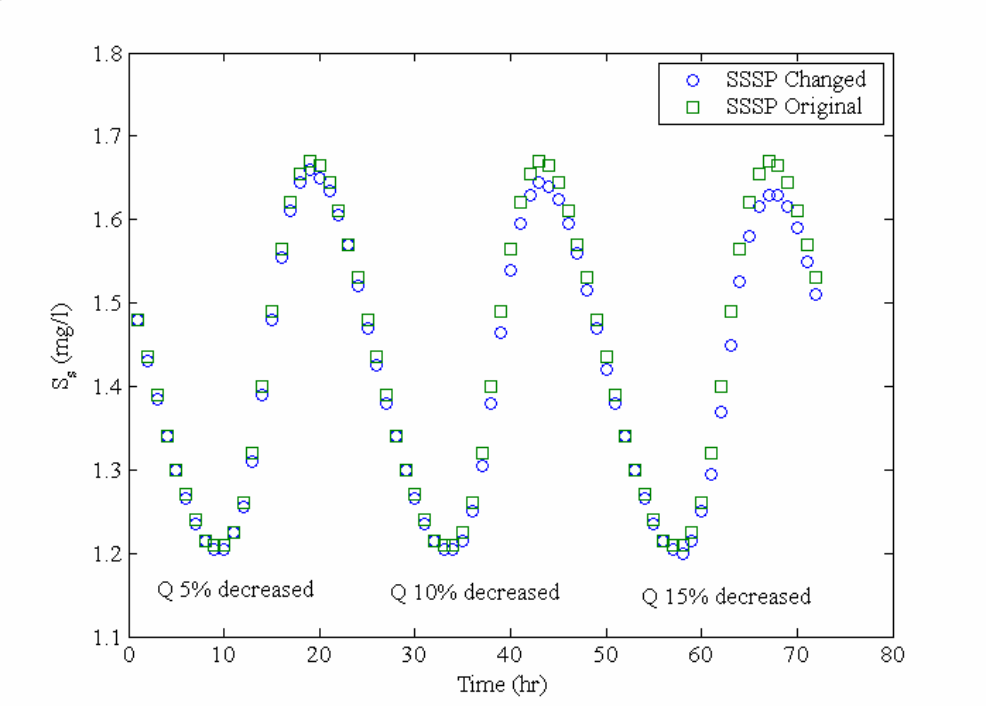


Figure 4.16 Sensitivity results of S_s for SSSP Hypothetical WWTP for changed $Q_{inf.}$

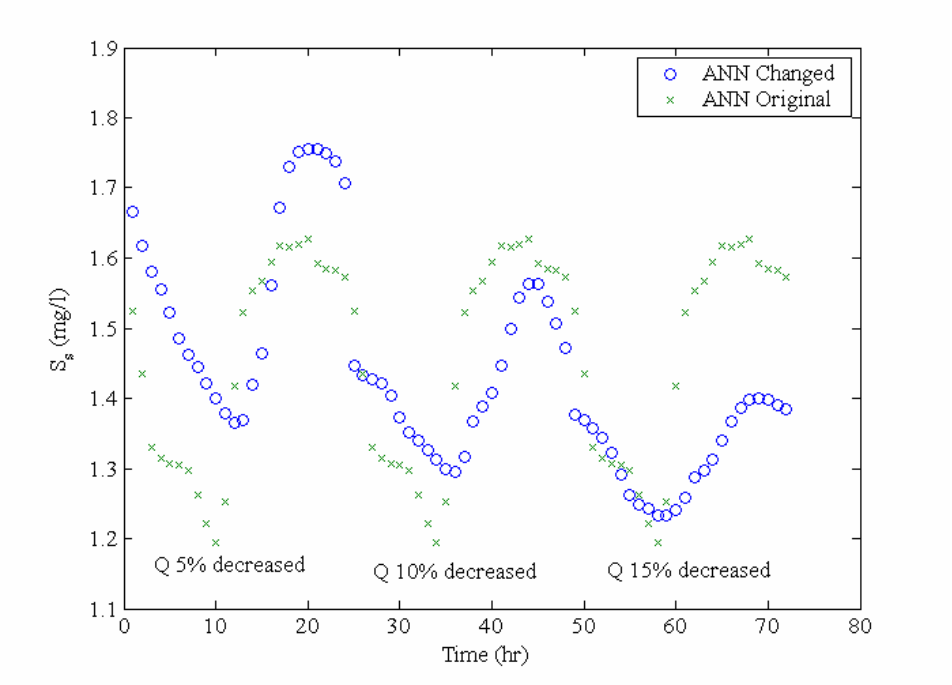


Figure 4.17 Sensitivity results of S_s for changed Q_{inf} in ANN Model (*trainlm, 10 HNs*).

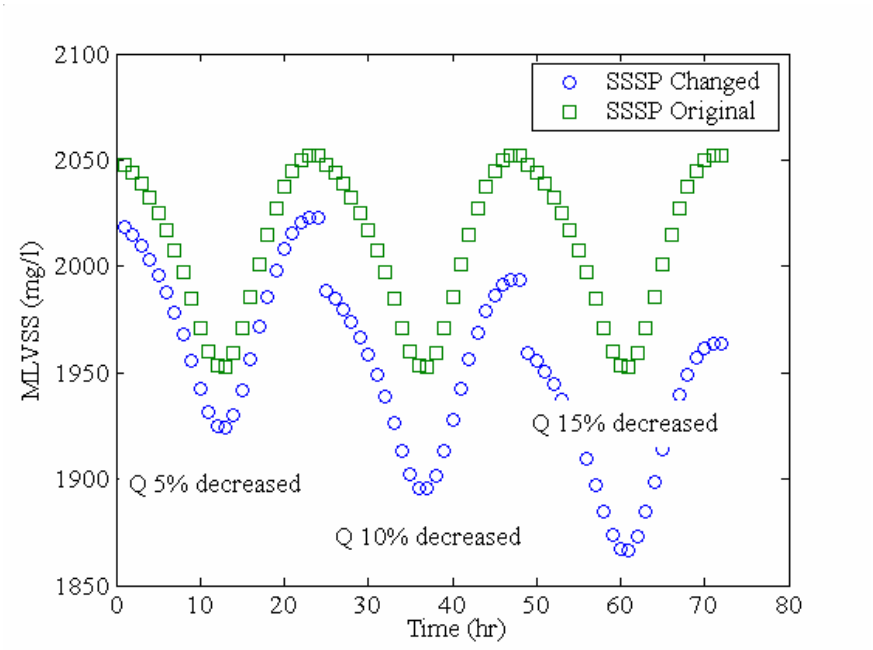


Figure 4.18 Sensitivity test results of MLVSS for SSSP Hypothetical WWTP for changing Q_{inf}.

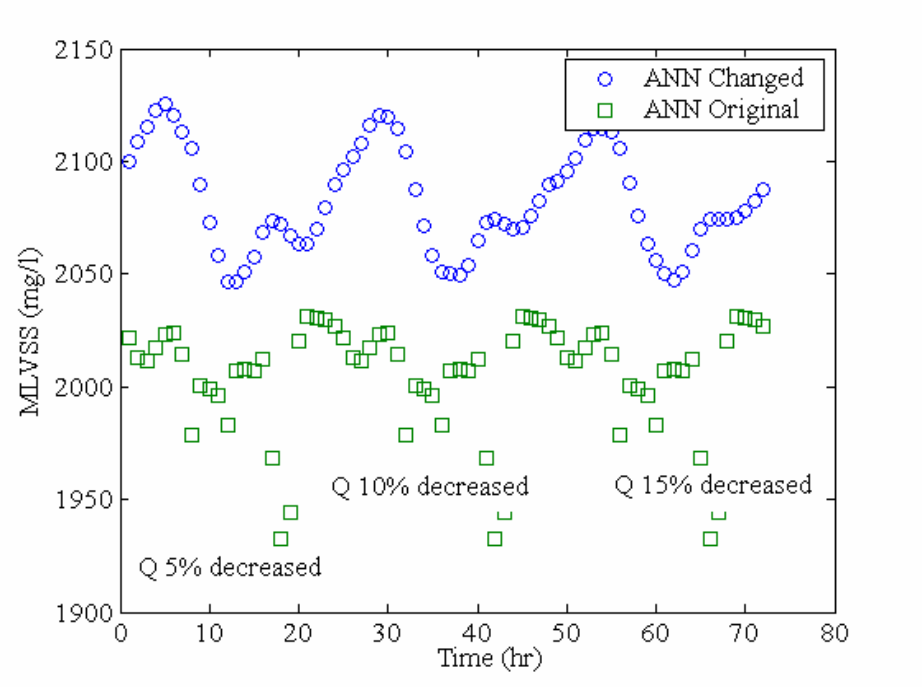


Figure 4.19 Sensitivity results of MLVSS for changed Q_{inf} in ANN Model (*trainlm, 10 HNs*).

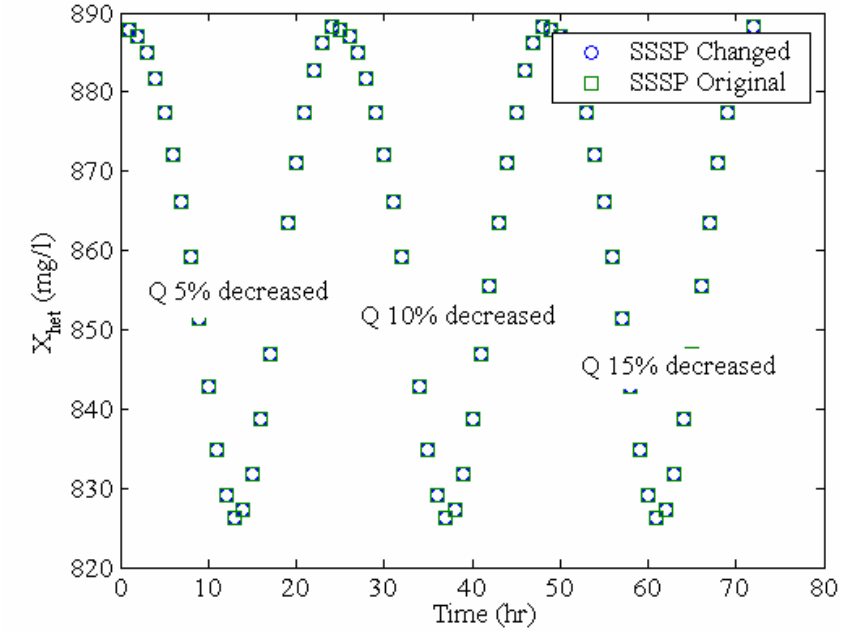


Figure 4.20 Sensitivity results of X_{het} for SSSP Hypothetical WWTP for changed X_i.

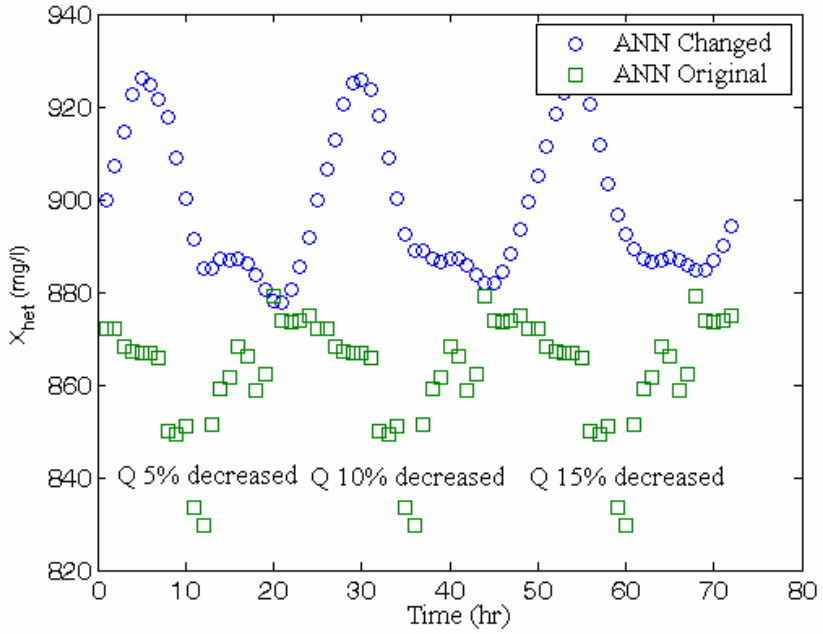


Figure 4.21 Sensitivity results of X_{het} for changed X_i in ANN Model (*trainlm, 10 HNs*).

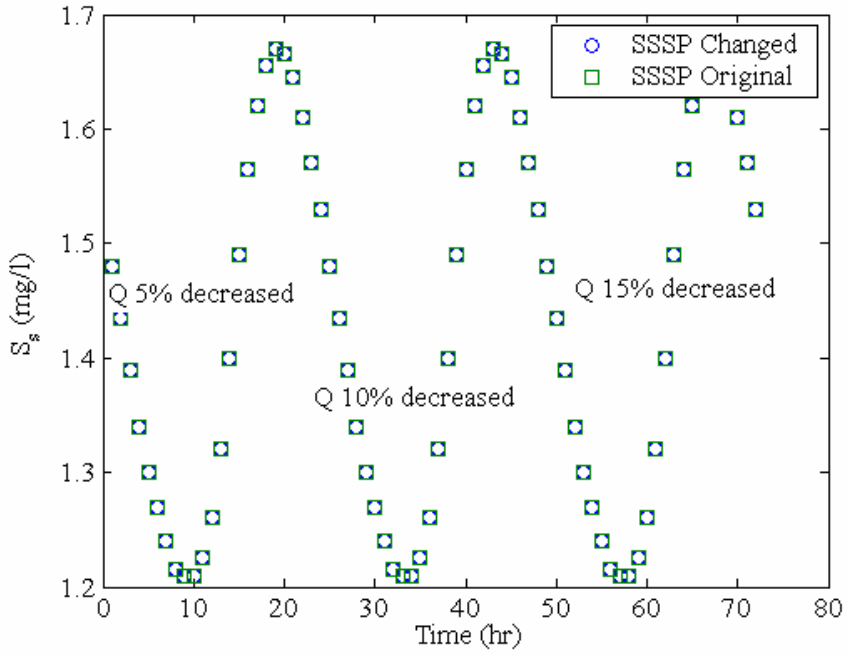


Figure 4.22 Sensitivity results of S_s for SSSP Hypothetical WWTP for changed X_i.

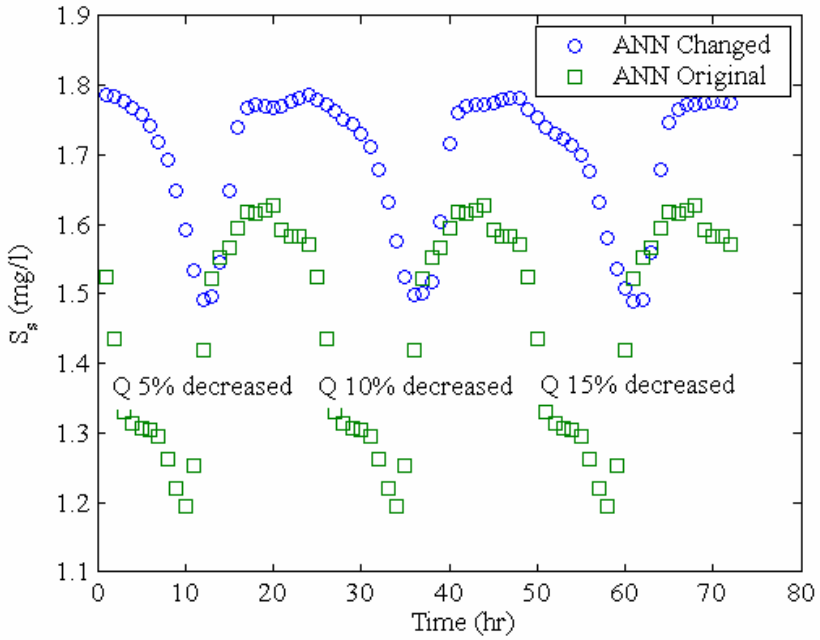


Figure 4.23 Sensitivity results of S_s for changed X_i in ANN Model (*trainlm, 10 HNs*).

4.3. ANN Modeling Studies with İskenderun Wastewater Treatment Plant (*IskWTP*) Data

4.3.1. IskWTP Data Preparation

Two different data sets were used for ANN modeling of IskWTP. These were belonging to the period from March 2002 to December 2002, and from January 2003 to May 2003. The first runs were made using the first set. However, the ANN models developed using this data set gave poor predictions. The highest correlation obtained was about 0.35. Then, the second set of data was used for model development.

In the modeling process, 9 of the system variables were used to build an ANN model. Also various combinations of the data were used in the model development process. System variables that were used in the modeling process were solids retention time (θ_c), influent flow rate (Q_{inf}), influent pH, influent water temperature (T_{inf}), influent COD concentration; MLSS, effluent COD, effluent TSS and sludge production rate from the primary sedimentation tank. These variables, singly or in combinations, were used to predict effluent COD concentration of the treated water from the treatment plant. Numerous combinations of variables were used and hundreds of models were developed and trained to see the efficacy of the prediction. Only those models resulting in high efficacy will be presented here.

Preparation of data was executed by excluding blank values from the original data set. Initially the raw data was composed of approximately 5 months of daily measurements, excluding Sundays, and summing up to 108 days. There were blanks in the data. Rows of data having blanks were removed completely from the set. For example, number of points used in ANN model for the three variable combinations, namely, effluent total suspended solids, MLSS of primary sedimentation tank and influent flow rate, was 99; where 9 rows of data containing blanks in any of the three variables were discarded.

4.3.2. IskWTP Data Preprocessing

After preparation of the data for the model development, preprocessing was carried out to assign all the variables equal weights in the weight update process, particularly when using a non-linear transfer function. The preprocessing was established by conversion of the input and output data into the range [0 1] or [-1 +1].

This conversion was done for all the points in the data as follows:

For [0 1] range;

$$X_i = \frac{x_i - x_{\min}}{x_{\max} - x_{\min}} \tag{4.1}$$

and for [-1 +1] range,

$$X_i = 2 \times \frac{x_i - x_{\min}}{x_{\max} - x_{\min}} - 1 \tag{4.2}$$

Each variable in the data have to be supplied in equal weights to the ANN model by normalizing the input data when nonlinear transfer functions like *logsig, tansig* were being used. Therefore, the data have to be scaled into [0 1] or [-1 +1] range using Equations 4.1 and 4.2, respectively.

In runs with [-1 +1] range, no good results were obtained. In these runs, firstly the script with one hidden layer was tried. Then, the hidden neuron number was changed using the criterion defined by Hecht and Nielsen (1987). The highest correlation coefficients obtained in these runs were around ***0.4***.

Later, number of hidden layers was increased to 2. Using the same data and in the [0 1] range, the transfer function *logsig* and in the [-1 +1] range, the transfer function tansig were used. It is possible to use transfer function combinations in multilayer models by using a particular transfer function at one layer and another at different layer(s). Some of the possible combinations of these functions when using two hidden layers (tansig-tansig, logsig-logsig, tansig-purelin, … etc.).

4.3.3. IskWTP ANN Model Development

The MATLAB Script was used to construct ANN models automatically by using the data for IskWTP. The implementation of the script started with the determination of the combinations of the variables to be used together. Variable combinations used in model development process are given in Table 4.6. These combinations were tried

in the given order until a good fits to the actual data were obtained by visual judgment and by considering the correlation coefficient, R. When an acceptable fit was reached, this was further improved by grouping the variables giving the best results.

As can be seen in Table 4.6, the best fit to the effluent COD data was obtained with the combination number 25, yielding ***R=0.795***. Basing on this observation, the variables identified in combination 25 were tested further singly or in pairs to create new subsets to be used in the script, in search for improved results. The variable combinations tested are presented in Table 4.5.

Table 4.5 Set descriptions for Combinations 25 and 26.

Set No	Variable(s) used
1	MLSS only,
2	TSS_{eff} only,
3	MLSS and Q_{inf},
4	Q_{inf} and TSS_{eff},
5	Q_{inf}, TSS_{eff} and MLSS,
6	MLSS and TSS_{eff}.

Table 4.6 Combinations of variables used in individual runs of the script.

No	**Q_{inf}**	**pH_{inf}**	**T_{inf}**	**COD_{inf}**	**MLSS**	**TSS_{eff}**	**ΔX**	**θ_c**	**Best R**
1	✓	✓	✓	✓					0.411
2	✓	✓	✓						0.360
3	✓	✓	✓		✓				0.310
4	✓	✓	✓			✓			0.462
5		✓	✓	✓				✓	0.257
6		✓	✓					✓	0.223
7		✓	✓		✓			✓	0.207
8		✓	✓			✓		✓	0.211
9	✓	✓	✓	✓			✓		0.291
10	✓	✓	✓				✓		0.256
11	✓	✓	✓		✓		✓		0.302
12	✓	✓	✓			✓	✓		0.321
13	✓		✓	✓					0.451

Table 4.6. (continued).

14	✓		✓					0.421
15	✓		✓		✓			0.397
16	✓		✓			✓		0.459
17			✓	✓			✓	0.243
18			✓				✓	0.268
19			✓		✓		✓	0.267
20			✓			✓	✓	0.289
21	✓		✓	✓			✓	0.269
22	✓		✓				✓	0.244
23	✓		✓		✓		✓	0.201
24	✓		✓			✓	✓	0.231
25	✓				✓	✓		**0.795**
26	✓				✓	✓		**0.729**

In addition to the manual altering of the variable combinations, the script automatically alters the number of hidden neurons for improved outputs. The outputs here were the effluent COD predictions. All these runs were made for different hidden layers. In the *first run*, there was 1 hidden layer and the hidden neuron number was changed from 1 to 9. As described earlier in the Methods section, there are 13 training functions available in the MATLAB ANN Toolbox basing on backpropagation algorithm. The script uses these functions sequentially to build the ANN models (Table 3.3). The transfer functions of *tansig*, and *logsig* were tried in different script runs. The script did not generate regression graphs as none of the tested models could yield a correlation coefficient greater than *0.6*. Subsequently, the same procedure was applied using the script for ANNs with two hidden layers. In the latter runs using the script with two hidden layers; again the number of hidden neurons was changed from 1 to 9 for both hidden layers.

The best fitting ANN model was determined according to the highest correlation coefficient. The ANN model response, regression analysis, and training session graphics are given in Figures 4.24, 4.25, 4.26, respectively. In Figure 4.24, the first half of the graph includes the training data. The second half (after x = 37700) contains the validation and training data. The results of regression analysis are given

in Figure 4.25. The blue line on the graph gives A=T, representing the theoretically best *possible* fit and the red line represents the best fit.

The MSE (mean square error) for the best run in the training session is given in Figure 4.26. The training session was stopped at epoch 48, upon completion of the validation process. There were three rules to stop the training session, (1) reaching the goal, which was to bring the Mean Squared Error (MSE) to zero, (2) exceeding the maximum fail number, which is already discussed in Section 3.3.2, and (3) reaching the maximum number of epoch given (here it was 20,000). In the best run, the 2nd stopping criterion was utilized to stop the training session.

The ANN model was taken from the 25th script run for IskWTP (Table 4.6). The system variables used in this script run were, namely, influent flow rate, effluent TSS, and MLSS. A 99 daily data were used in the model development. The data was divided into three parts as training, validation and test sets. The first 50% (1-49th days) of the data was taken as the training data, 25% (50-74th days) was taken as the validation set that was used for validation of the direction of the error decrease during the training (parameter estimation) and the remaining (75-99th days) was taken as the test data. The 26th combination was the same as 25th; the difference being in that the data was not fed in chronological order.

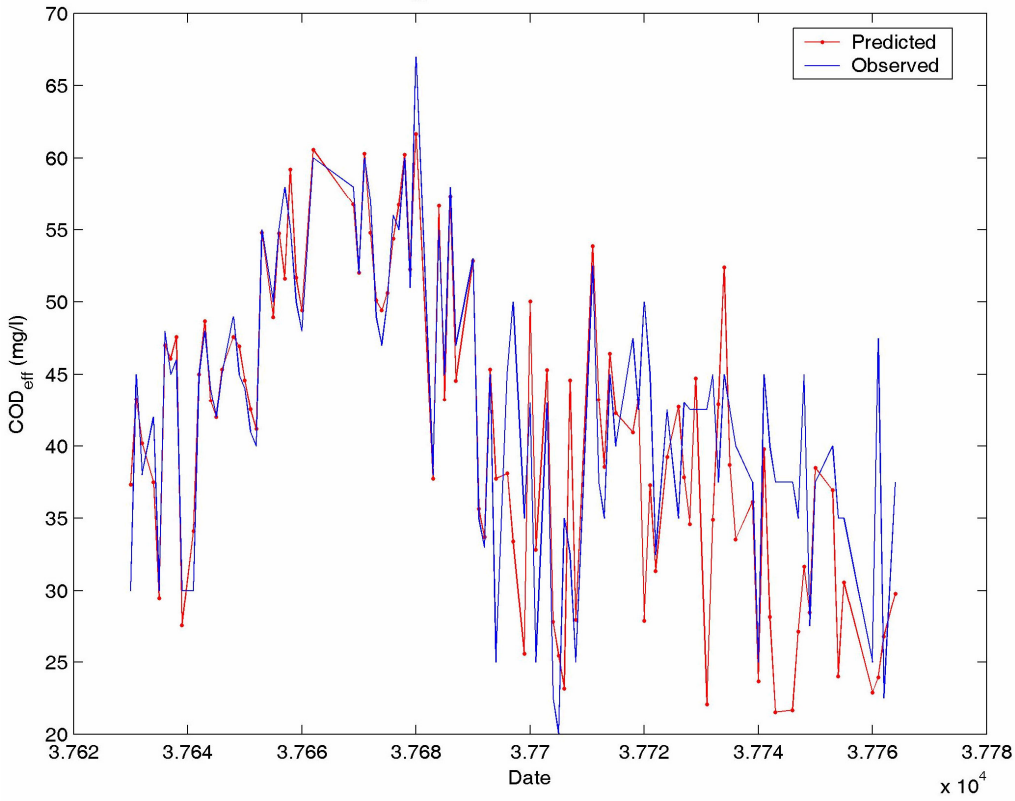


Figure 4.24 Prediction of COD in the best ANN model with R=0.795.

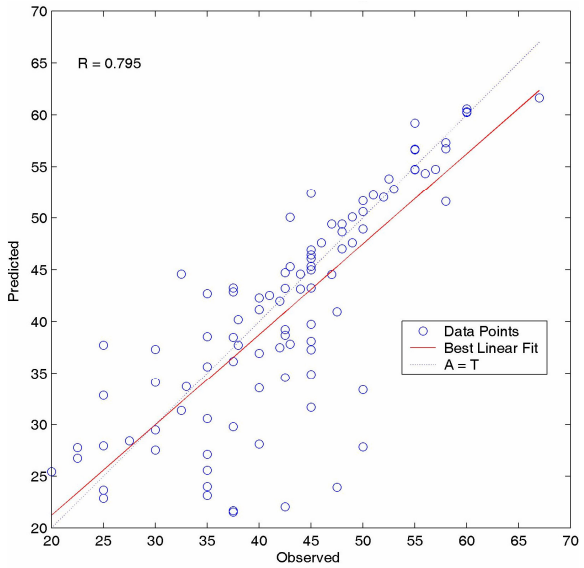


Figure 4.25 Regression analysis of the best ANN model.

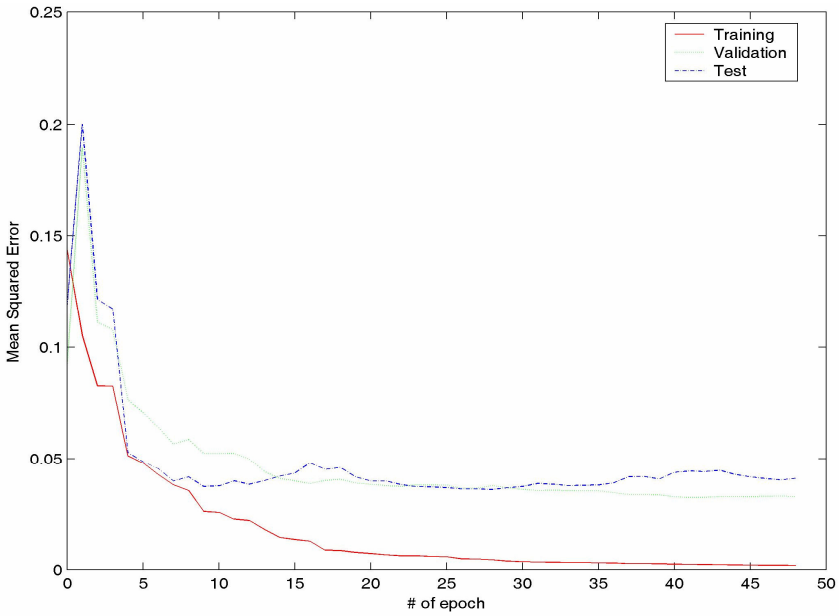


Figure 4.26 Prediction of COD in the best ANN model with R=0.795

It can be seen in Figures 24, 25, and 26 that the results obtained were fairly good. The best correlation coefficient obtained was ***0.795.*** Results could have been even better if the data used were more numerous and accurate. The data set used in this study included too many blanks which interrupted a continuous data input to the ANN model. The quality of daily data was unsure which increased uncertainty. Although it is known that ANN can cope with noisy and erroneous data well, the process parameters in biological wastewater treatment used in ANN modeling are numerous and relative error is often high in these. Therefore the combination of errors propagates during ANN modeling. Therefore, ideally the main purpose in ANN modeling would be to predict objective variables using the data from automatic sensors controlling the treatment plant. Random human error would be minimized by this.

The best results obtained using the MATLAB Script, are given in Tables 4.7 and 4.8. In these tables, name of the backpropagation algorithm, variable set

combination number (i.e. 1-26) from Table 4.6, the number of hidden neurons employed, and the correlation coefficient obtained are given collectively.

Table 4.7 The best results of 25th run of the script.

Training function	Set	HNs	R
trainbfg	6	4	0.673
traincgb	***5***	***6***	***0.795***
traincgb	6	6	0.694
trainlm	6	1	0.670
trainscg	6	6	0.668

Table 4.8 The best results of 26th run of the script.

Training function	Set	HNs	R
trainb	4	2	0.696
trainbfg	5	3	0.673
trainbfg	5	6	0.673
trainbr	5	3	0.691
traincgp	5	2	0.693
trainlm	4	4	0.729
trainlm	4	6	0.709
trainlm	4	7	0.684
trainrp	5	4	0.703
trainscg	4	4	0.669

The ANN modeling can be thought as a two step process. Firstly, the combination of variables giving the best result was taken for creating the new variable sets. In this case variables identified in the 25th set in Table 4.7 were used and new combinations were tried using these identified variables. The 26th set (Table 4.8) was identical to the 25th with the difference in the order of data fed to the ANN model. In the 26th set, data was fed randomly whereas in 25th a chronological order was followed.

4.4. ANN Modeling Studies with Ankara Central Wastewater Treatment Plant (ACWTP) Data

4.4.1. ACWTP Data Preparation

The ACWTP data was prepared firstly by determining the variables to be used in the ANN model development. The blanks in the data set were excluded as before. When choosing the parameters that will be used for ANN modeling, variables such as organic loading, solids retention time, MLSS, water and air temperatures, alkalinity and pH, were selected by considering the ASP kinetic. Then in a second attempt, the solids retention time and organic loading in the first set at above were replaced by the influent flow rate, influent COD concentration and return activated sludge flow rates.

Other trials have also been made by smoothing out the data by using higher order polynomial equations (up to 6^{th} degree) for every variable to obtain an optimal ANN model that can predict effluent COD concentrations reasonably accurate. The polynomials were fitted to the data set for each variable. Moreover, in a later attempt, data were divided into subsets considering the seasons of the year and each subset was trained, verified, and tested with the parsed data. However, no significant fit could be obtained in these trials.

Monthly data were parsed by using Genetic Algorithm program, PGAPack, into three to form the components for training, validation and test sets for the ANN models. The code that divides the data set into three equally averaged sets is given in Appendix D and the formula used in minimization in Equation 4.2.

4.4.2. ACWTP Data Preprocessing

The data to be used in ANN modeling was initially normalized in the [0 1] or [-1 +1] form by using each variable's minimum and maximum values and by using the given formula (Equation 4.2). Moreover data was normalized around its mean value with reference to the standard deviation of the set, as follows:

$$X_i = \frac{x_i - \mu}{\sigma} \tag{4.3}$$

where

μ = mean value of the variable to be normalized,

σ = standard deviation of the variable to be normalized.

The three forms of normalized data were run separately in order to obtain a higher match to the observed data. These trials were unfruitful, therefore will not be discussed here extensively.

4.4.3. ACWTP ANN Model Development

After preprocessing the data for model development, effective variables on the system performance were selected (25^{th} combination in Table 4.6). As discussed earlier in Section 4.4.1, ANN modeling using the selected cardinal variables of ASP kinetics, such as SRT, organic loading; yielded very poor fits with R around ***0.4***. These variable sets were therefore abandoned and replaced by those identified in 25^{th} combination in Table 4.6 in search for better fits.

The newly selected variables were used in the script to build the ANN models for the system. At first, one hidden layer was used with *logsig* transfer function, and by changing the number of hidden neurons from 1 to 12. Data were parsed in two different percentages for ACWTP modeling. Namely, 50% of data were used for training, 25% for validation and 25% for the test set and in the second group 34% for training, 33% for validation, and 33% for test. The data which were normalized

in three different forms were subsequently used for ANN modeling. Any changes made on the model format were implemented to the three forms of normalized data runs. For example, changing the transfer function on one set of normalized data lead to applying this to the other two normalized data sets

Table 4.9 Combinations of variables selected for ANN model building using the script.

Combo.	Organic Load	θ_c	Turbidity	TSS	T_{water}	T_{air}	Alk.	pH	R
1		✓							0.136
2		✓	✓						0.191
3		✓		✓					0.211
4		✓			✓				0.179
5		✓				✓			0.165
6		✓					✓		0.176
7		✓						✓	0.187
8	✓								0.120
9	✓	✓							0.143
10	✓	✓	✓						0.155
11	✓	✓		✓					0.324
12	✓	✓			✓				0.201
13	✓	✓				✓			0.186
14	✓	✓					✓		0.165
15	✓	✓						✓	0.197
16	✓		✓						0.187
17	✓			✓					0.200
18	✓				✓				0.169
19	✓					✓			0.145
20	✓						✓		0.134
21	✓							✓	0.121

Initially the best result obtained was (with Organic Load, θ_c, and Turbidity variable combination) in run with two hidden layers which produced a correlation coefficient of ***0.32*** using *logsig* transfer function, normalized into [0 1] range (Table 4.9). Thus, a total of twelve runs were made to improve the fit. All four types of data

normalizations ([+1 -1], etc.) in two data parse groups, and in two training functions (*logsi, tansig*) were tested. The R value reduced to ***0.30*** when *tansig* was used.

The script was slightly modified to build ANN models of two hidden layers with this data. All other criteria in the script were kept identical to that with one hidden layer but an additional transfer function for the second layer was added. In the runs with two layers only up to 9 hidden neurons could be used as computer memory capacity was exceeded beyond this point and further runs could not be implemented. The total transfer function combinations tested for the two hidden layers were four in number; namely, tansig-tansig and logsig-logsig. However, no appreciable correlation could be obtained in these trials and this approach was therefore aborted.

Following the failure in trials with two hidden layers and the choice of parameters on basic ASP kinetics, it was decided to select available operational parameters such as "influent flow rate, return activated sludge flow rate and influent COD concentration" instead of organic loading and solids retention time. The new variable set used in the model development process is given in Table 4.10. The parameter combinations shown in Table 4.10 were tested by using the script. The best correlation coefficient obtained was ***0.56***.

Table 4.10 Combinations of variables used with selected operational variables.

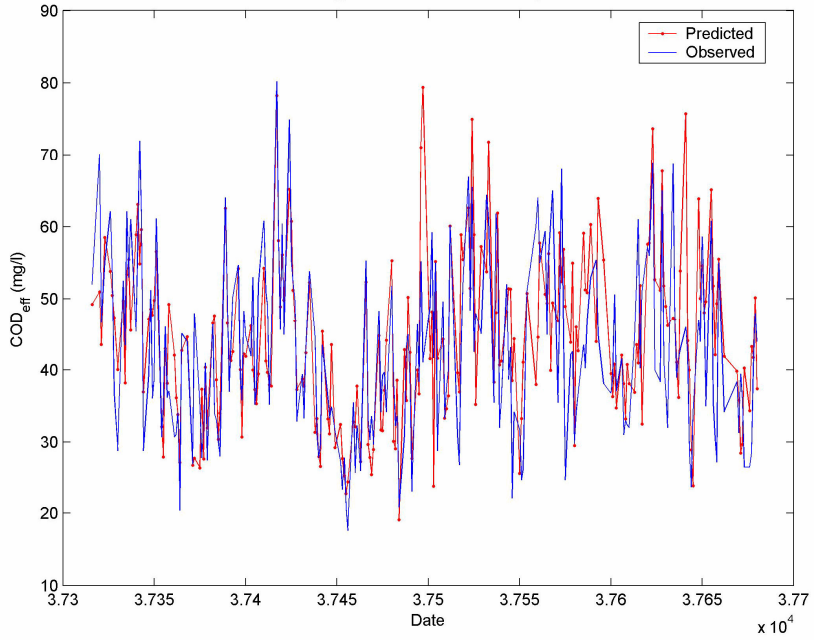
Combo.	Q_{1inf}	COD_{inf}	pH	Alk.	Q_{ret}	Turbidity	TSS	T_{water}	T_{air}	R
1		✓	✓						✓	0.465
2		✓		✓					✓	0.470
3		✓			✓				✓	0.407
4		✓				✓			✓	0.556
5		✓					✓		✓	0.511
6	✓	✓	✓						✓	0.504
7	✓	✓		✓					✓	0.470
8	✓	✓			✓				✓	0.380
9	✓	✓				✓			✓	0.457
10	✓	✓					✓		✓	0.504

The poor fit with *R=0.56* suggested that other remaining variable combinations also be tested. In order to implicate the correct variables for ANN combinations a regression analyses between the possible input variables and the outputs (COD) was carried out. The resultant correlation matrix is given in Table 4.12 and combinations of selected variables after regression analysis are given in Table 4.11.

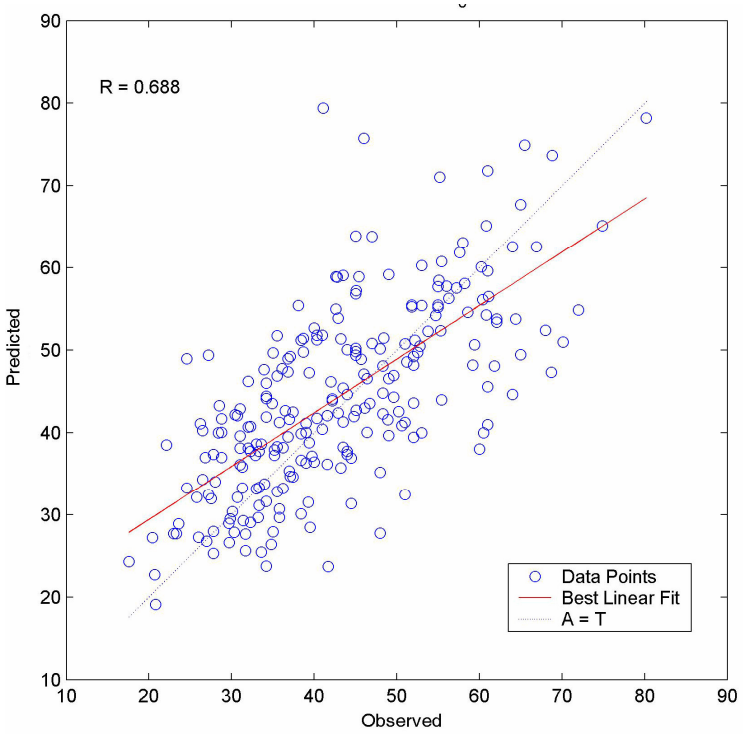
Table 4.11 Combinations of variables determined with the regression analysis used in the individual runs of the script.

Combo.	$COD_{effprimarysed}$	TSS_{eff}	T_{air}	T_{water}
1	✔	✔	✔	
2	✓	✓		✓
3	✓	✓	✓	✓
4	✓	✓		

The best correlation coefficient obtained with these variable combinations in Table 4.11 was ***0.688*** (***from Combo. 1***) which corresponded to the best result obtained for ACWTP in all the models developed. Graphical outputs for model predictions, regression analysis, and training session are given in Figures 4.27, 4.28, 4.29.



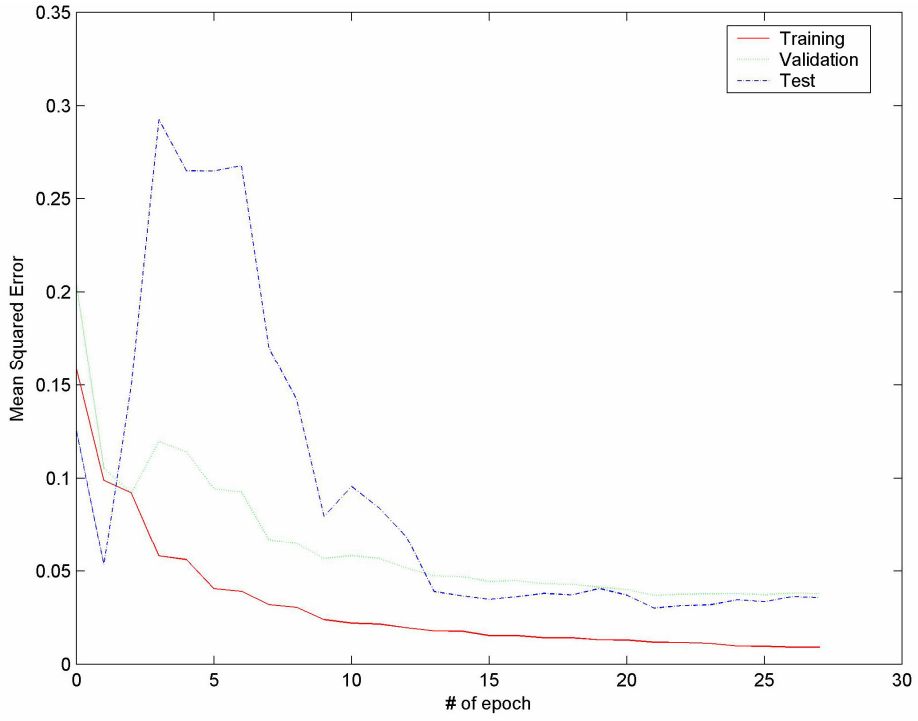
Figures 4.27 Best model developed (*traincgb*, *4 HNs*) for ACWTP.



Figures 4.28 Regression analysis for the best model developed for ACWTP.

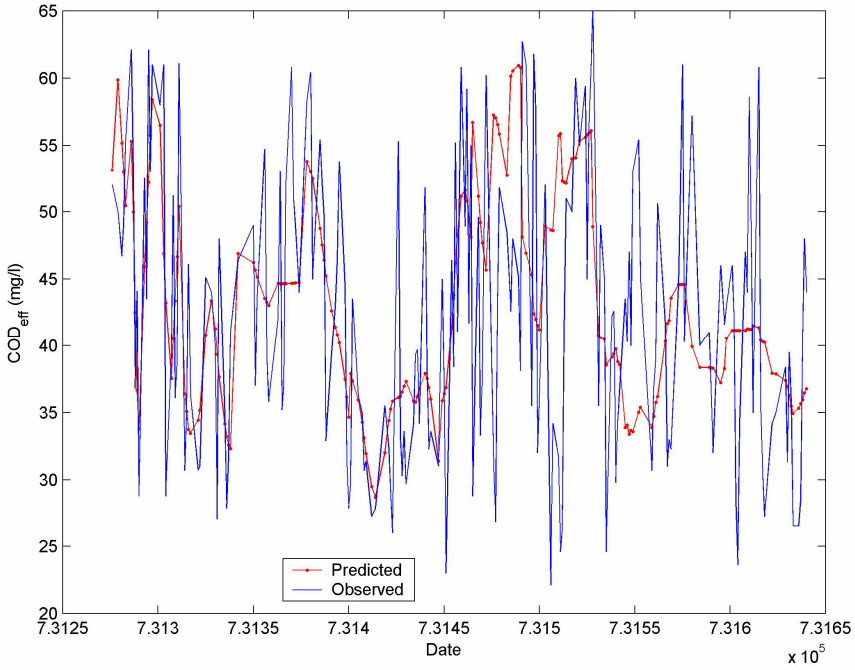
Table 4.12 Variable Correlation matrix.

	Q_{1inf}	COD_{inf}	θ_{cr1}	Q_{ret}	*Turbidity*	*TSS*	T_{su}	*pH*	*Alkalinity*	COD_{eff}
Q_{1inf}	1.000									
COD_{inf}	-0.228	1.000								
θ_{cr1}	0.177	-0.092	1.000							
Q_{ret}	0.428	-0.274	0.494	1.000						
Turbidity	-0.004	0.383	-0.107	-0.201	1.000					
TSS	-0.223	0.463	-0.178	-0.301	0.529	1.000				
T_{su}	-0.375	0.135	-0.637	-0.567	0.298	0.232	1.000			
pH	0.293	-0.331	0.335	0.394	-0.317	-0.317	-0.585	1.000		
Alkalinity	-0.188	0.137	0.347	0.031	-0.220	-0.092	-0.490	0.198	1.000	
COD_{eff}	***-0.018***	***0.310***	***-0.070***	***-0.152***	***0.075***	***0.048***	***-0.044***	***0.048***	***0.129***	***1.000***



Figures 4.29 training session for the best model developed for ACWTP.

After all these trials, it was seen that the highest correlation coefficient found (*R= 0.688*) was not satisfactory in modeling the treatment plant under consideration and other methods of fit were tried. In these trials input data were smoothened by creating approximate polynomial equations for each variable that will be used for the prediction of effluent COD concentration. However, the ANN models developed after smoothening seemed to have captured the trend of the mean values but extremely volatile character of the COD output data prevented a close match as can be seen in Figure 4.30.



Figures 4.30 Prediction with polynomial data using two hidden layers for ACWTP.

CHAPTER V

CONCLUSIONS

The following conclusions can be drawn from this study:

- Ideally ANN could accurately model activated sludge process, as indicated by simultaneous studies carried out using the SSSP program.
- The sensitivity of the ANN model is also acceptable as compared with the SSSP program response.
- Regarding the actual data, the accuracy of the ANN model deteriorates owing to the errors in data production.
- In the case of actual data from IskWTP, the best fit obtained by the ANN model yielded a R value of 0.795, which can be considered very high with such a noisy data.
- The variable input combination was Q_{inf}, TSS_{effl}, MLVSS in the best run with R=0.795 for effluent COD prediction in IskWTP. However, use of TSS_{eff} may not be meaningful if this model is to be used for the control of the WWTP. In this run 2 hidden layers, 6 HN and *logsig* transfer function were used.
- In the case of ACWTP, the R value obtained was 0.688, where accuracy of fit is debatable. The study of model building can be repeated using a new set of data that was measured for the specific purpose of ANN modeling..
- With noise-free data, such as those supplied by the SSSP program, even with one hidden layer and using three selected variables, highly accurate predictions in any of the three objective variables were obtained. The R values for MLVSS, X_{HET} and SS were greater than 0.98.
- It is seen that noise in the data caused miscalculation of the fundamental operational parameters of the activated sludge process and resulted in loss of both sensitivity and precision. Therefore ANN modeling should best be used in association with automated data logging equipment. In this case even

systematic bias that would be produced by the instrumentation would not appreciably impact the precision of the predictions. Whereas manual data produced may contain both random and systematic errors which result in great loss of precision.

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APPENDIX A

SSSP Simulation Program Default Dynamic Data Figures & Tables

A.1. SSSP Simulation Program Default Influent Data

Table A.1. Input Data given in the SSSP Program.

Time	Input			Normalized Input		
	Flow	**Xi**	**Sol. Org.**	**Flow**	**Xi**	**Sol. Org.**
0	725	30.1	98.9	0.27281	0.45477	0.45441
1	594	27.7	91.0	0.15447	0.39447	0.39387
2	524	21.7	71.2	0.09124	0.24372	0.24215
3	453	19.2	63.2	0.02710	0.18090	0.18084
4	423	16.9	55.4	0.00000	0.12312	0.12107
5	423	15.6	51.4	0.00000	0.09045	0.09042
6	503	13.2	43.5	0.07227	0.03015	0.02989
7	725	12.0	39.6	0.27281	0.00000	0.00000
8	1128	12.0	39.6	0.63686	0.00000	0.00000
9	1409	15.6	51.4	0.89070	0.09045	0.09042
10	1460	24.1	79.1	0.93677	0.30402	0.30268
11	1440	36.7	120.6	0.91870	0.62060	0.62069
12	1470	43.3	142.4	0.94580	0.78643	0.78774
13	1530	48.2	158.2	1.00000	0.90955	0.90881
14	1510	48.8	160.2	0.98193	0.92462	0.92414
15	1420	48.2	158.2	0.90063	0.90955	0.90881
16	1329	51.8	170.1	0.81843	1.00000	1.00000
17	1208	51.2	168.1	0.70912	0.98492	0.98467
18	1097	48.2	158.2	0.60885	0.90955	0.90881
19	1027	41.5	136.4	0.54562	0.74121	0.74176
20	1007	36.1	118.7	0.52755	0.60553	0.60613
21	926	34.3	112.7	0.45438	0.56030	0.56015
22	886	33.7	110.8	0.41825	0.54523	0.54559
23	785	32.5	106.8	0.32701	0.51508	0.51494
Min	**423**	**12.0**	**39.6**	**0.00000**	**0.00000**	**0.00000**
Max	**1530**	**51.8**	**170.1**	**1.00000**	**1.00000**	**1.00000**

A.2. Effluent SSSP response to given influent data.

Table A.2. Output obtained from the SSSP simulation program using the input data.

Time	Output			Normalized Output		
	MLVSS	**Xhet**	**Ss**	**MLVSS**	**Xhet**	**Ss**
0	2047.73	887.840	1.480	0.95340	0.99195	0.58696
1	2044.00	886.990	1.435	0.91594	0.97826	0.48913
2	2038.89	884.900	1.390	0.86457	0.94460	0.39130
3	2032.58	881.665	1.340	0.80120	0.89250	0.28261
4	2025.23	877.390	1.300	0.72738	0.82366	0.19565
5	2016.96	872.185	1.270	0.64437	0.73983	0.13043
6	2007.71	866.145	1.240	0.55142	0.64256	0.06522
7	1997.09	859.235	1.215	0.44476	0.53128	0.01087
8	1984.58	851.325	1.210	0.31912	0.40390	0.00000
9	1971.27	842.800	1.210	0.18550	0.26661	0.00000
10	1960.06	834.935	1.225	0.07291	0.13995	0.03261
11	1953.40	829.060	1.260	0.00603	0.04533	0.10870
12	1952.80	826.245	1.320	0.00000	0.00000	0.23913
13	1958.92	827.195	1.400	0.06146	0.01530	0.41304
14	1970.80	831.760	1.490	0.18073	0.08882	0.60870
15	1985.57	838.765	1.565	0.32906	0.20163	0.77174
16	2000.72	846.940	1.620	0.48127	0.33328	0.89130
17	2014.92	855.415	1.655	0.62383	0.46976	0.96739
18	2027.25	863.545	1.670	0.74766	0.60069	1.00000
19	2037.34	870.990	1.665	0.84905	0.72059	0.98913
20	2045.11	877.510	1.645	0.92709	0.82559	0.94565
21	2050.07	882.660	1.610	0.97690	0.90853	0.86957
22	2052.37	886.285	1.570	1.00000	0.96691	0.78261
23	2052.32	888.340	1.530	0.99950	1.00000	0.69565
Min:	**1952.80**	**826.245**	**1.210**	**0.00000**	**0.00000**	**0.00000**
Max:	**2052.37**	**888.340**	**1.670**	**1.00000**	**1.00000**	**1.00000**

A.3. ANN Manual Model Run Results for SSSP Simulation Program

Table A.3. MLVSS, ANN model prediction results.

Time	MLVSS					
	Real	Trial 1	Trial 2	Trial 3	Trial 4	Trial 5
0	2047.730	2042.931	2049.005	2030.873	2044.992	2045.002
1	2044.000	2048.736	2049.482	2035.762	2045.609	2045.639
2	2038.885	2051.763	2049.463	2037.385	2037.225	2037.205
3	2032.575	2052.091	2049.532	2039.406	2035.463	2035.433
4	2025.225	2052.171	2049.502	2040.193	2029.160	2029.120
5	2016.960	2052.191	2049.443	2039.874	2022.838	2022.818
6	2007.705	2052.171	2048.935	2036.518	2000.962	2001.032
8	1984.575	2028.374	1979.315	1986.196	1983.945	1983.955
9	1971.270	1963.245	1961.214	1963.464	1970.962	1971.011
10	1960.060	1964.659	1964.031	1965.286	1961.363	1961.363
11	1953.400	1984.792	1966.790	1976.667	1958.466	1958.436
12	1952.800	1977.683	1963.086	1979.724	1960.995	1960.975
14	1970.795	1966.252	1967.337	1981.108	1971.330	1971.320
15	1985.565	1973.929	1977.653	1990.218	1980.958	1980.899
16	2000.720	1974.695	2002.884	2002.595	2001.868	2001.958
17	2014.915	1981.635	2013.129	2012.114	2012.194	2012.263
18	2027.245	1996.780	2018.128	2017.919	2029.887	2029.807
20	2045.110	2030.046	2042.592	2017.730	2045.739	2045.749
21	2050.070	2033.701	2046.217	2022.021	2046.724	2046.764
22	2052.370	2035.264	2047.143	2024.003	2046.943	2046.973

Table A.4. Heterotrophic Biomass, ANN model prediction results.

Time	Xhet					
	Real	Trial 1	Trial 2	Trial 3	Trial 4	Trial 5
0	887.840	826.593	881.932	871.394	885.111	885.117
1	886.990	826.531	882.677	871.463	885.831	885.844
2	884.900	826.475	882.503	871.003	882.565	882.553
3	881.665	826.450	882.584	870.649	881.826	881.808
4	877.390	826.444	882.522	870.376	878.995	878.970
5	872.185	826.444	882.429	870.376	875.946	875.927
6	866.145	826.462	881.671	870.469	863.682	863.713
8	851.325	828.841	838.807	847.022	852.319	852.312

Table A.4.(continued).

9	842.800	836.186	831.057	831.728	843.420	843.439
10	834.935	833.237	832.051	833.094	831.386	831.355
11	829.060	829.362	830.995	841.899	827.903	827.884
12	826.245	834.286	829.443	844.793	828.940	828.928
14	831.760	852.039	832.007	846.575	833.212	833.181
15	838.765	843.663	835.944	853.244	837.360	837.310
16	846.940	848.655	853.877	862.043	848.487	848.506
17	855.415	842.930	860.664	867.203	853.952	853.995
18	863.545	833.243	860.782	869.469	863.986	863.986
20	877.510	826.816	872.984	868.196	878.535	878.504
21	882.660	826.717	877.790	869.656	882.435	882.435
22	886.285	826.686	879.131	870.233	883.615	883.621

Table A.5. Suspended Solids, ANN model prediction results.

Time	Ss					
	Real	Trial 1	Trial 2	Trial 3	Trial 4	Trial 5
0	1.480	1.226	1.670	1.511	1.483	1.483
1	1.435	1.221	1.670	1.519	1.481	1.481
2	1.390	1.215	1.670	1.519	1.349	1.349
3	1.340	1.214	1.670	1.521	1.332	1.332
4	1.300	1.213	1.670	1.521	1.292	1.292
5	1.270	1.213	1.670	1.520	1.268	1.268
6	1.240	1.213	1.670	1.514	1.229	1.229
8	1.210	1.216	1.670	1.334	1.218	1.218
9	1.210	1.219	1.670	1.245	1.216	1.216
10	1.225	1.222	1.670	1.252	1.224	1.224
11	1.260	1.236	1.669	1.300	1.273	1.273
12	1.320	1.348	1.666	1.314	1.342	1.342
14	1.490	1.589	1.657	1.320	1.486	1.487
15	1.565	1.567	1.661	1.362	1.550	1.550
16	1.620	1.630	1.644	1.420	1.624	1.624
17	1.655	1.619	1.645	1.461	1.637	1.637
18	1.670	1.527	1.660	1.483	1.649	1.649
20	1.645	1.235	1.670	1.476	1.627	1.626
21	1.610	1.232	1.670	1.489	1.600	1.600
22	1.570	1.231	1.670	1.495	1.586	1.587

APPENDIX B

SSSP Simulation Results of Trial5: Prediction and Regression Graphs

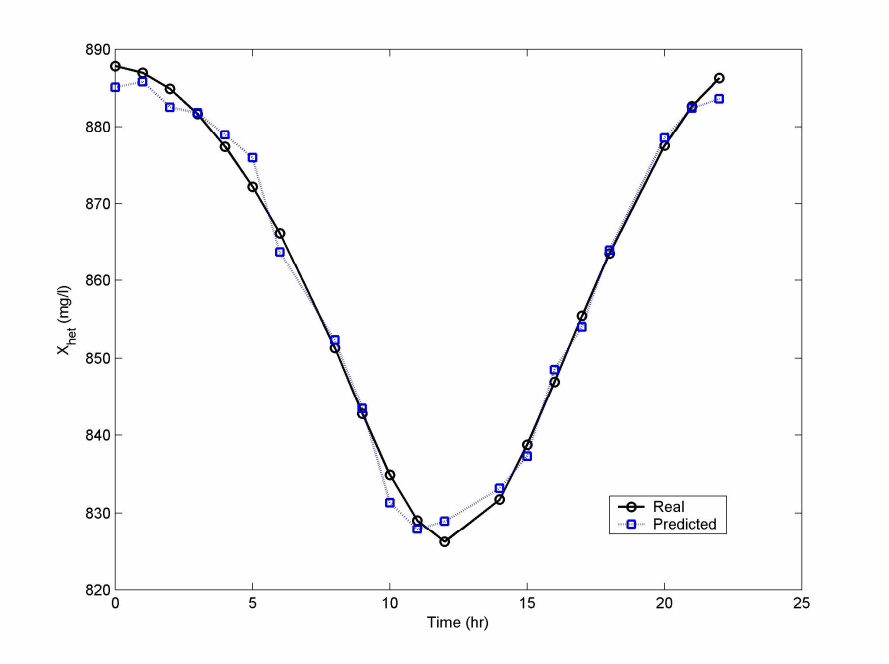

Figure B.1 ANN Model run results for X_{het} predictions for Trial5.

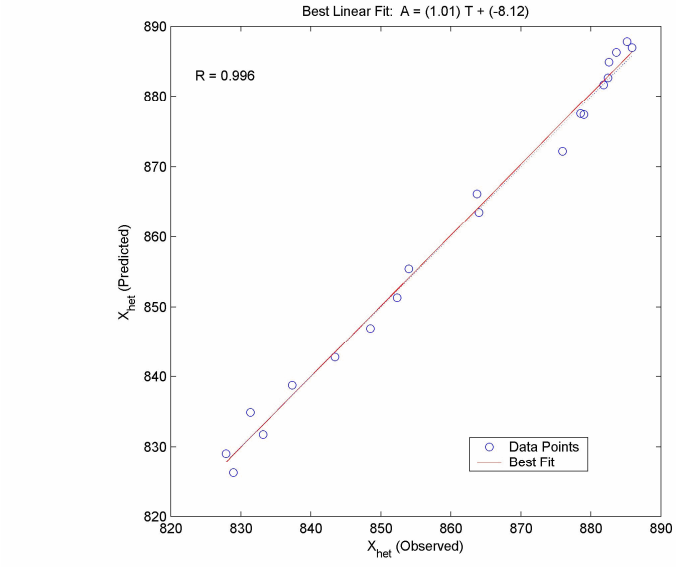

Figure B.2 Regression analysis result of X_{het} variable for Trial5 ANN model.

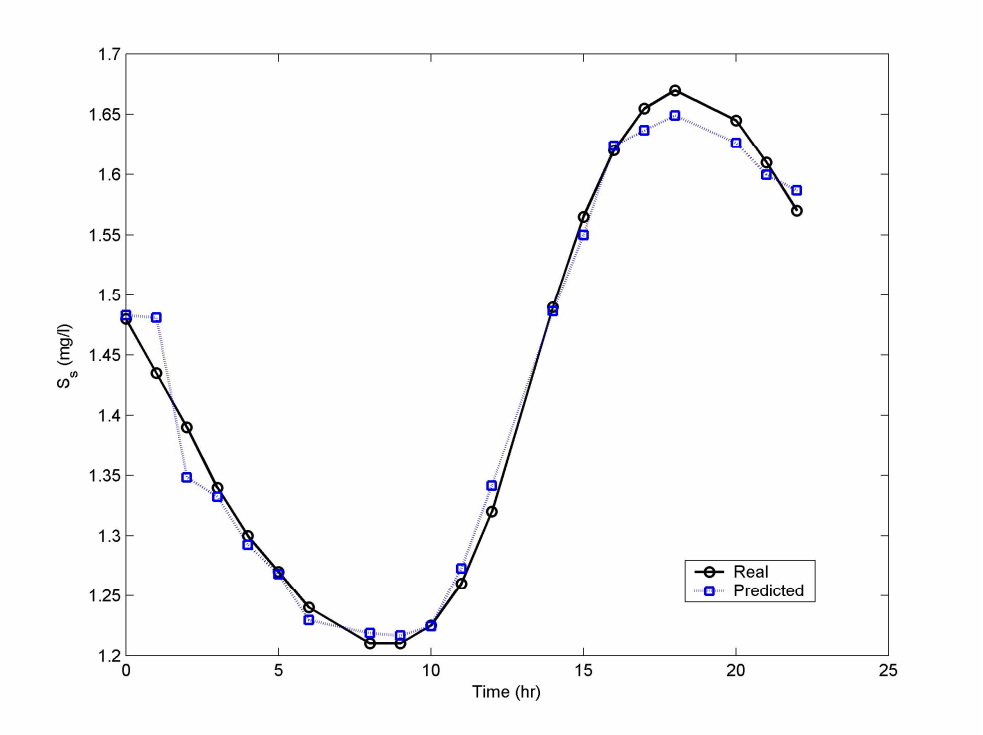

Figure B.3 ANN Model run results for S_s predictions for Trial5.

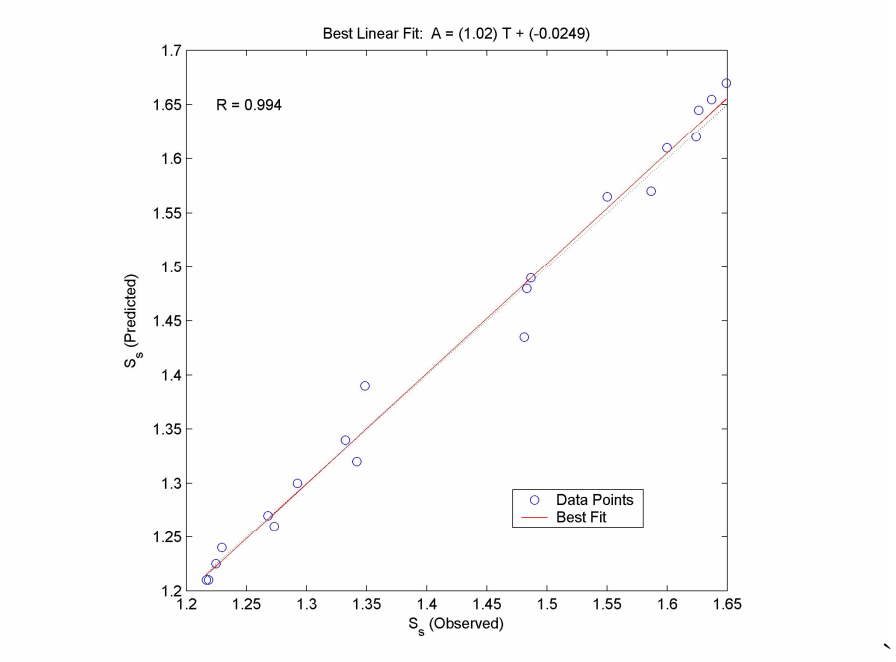

Figure B.4 Regression analysis result of Ss variable for Trial5 ANN model.

Table B.1 Regression analyses results made with the results of script developed including validation data.

training Function	Hidden Neuron #	MLVSS	S_s	X_{het}
trainb	2	-0.005	0.853	0.756
	8	0.816	0.749	0.277
	9	0.386	0.942	0.752
trainbfg	3	0.776	0.973	0.535
	9	0.752	0.792	0.868
	10	0.805	0.893	-0.596
trainbr	*3*	*0.971*	*0.942*	*0.938*
	4	0.886	0.908	0.932
	5	*0.954*	*0.922*	*0.943*
	7	0.838	0.882	0.940
	9	*0.955*	*0.969*	*0.948*
	10	0.928	0.920	0.940
traincgb	6	0.841	0.985	0.265
	7	0.874	0.983	0.942
	9	0.943	0.863	0.970
traıncgb	10	0.895	0.901	0.790
traincgf	4	0.936	0.949	0.650
	9	0.905	0.945	0.490
traincgp	2	0.873	0.949	0.601
	6	0.951	0.926	0.681
	7	0.866	0.808	0.926
	10	0.890	0.894	0.960
traingd	-	-	-	-
traingda	*8*	*0.946*	*0.992*	*0.864*
traingdm	-	-	-	-
traingdx	6	0.679	0.930	0.960
trainlm	6	0.090	0.970	0.959
	9	*0.908*	*0.989*	*0.988*
	10	0.645	0.914	0.981
trainoss	10	0.977	0.956	0.154
trainrp	6	0.683	0.959	0.877
	7	0.588	0.821	-0.848
	8	0.476	0.968	0.937
	10	*0.920*	*0.947*	*0.870*
trainscg	2	-0.764	0.490	0.139
	3	0.736	0.844	-0.412

Table B.1 (Continued).

trainscg	4	0.511	0.238	-0.470
	5	0.925	0.697	-0.079
trainscg	7	0.753	0.959	0.553
	9	0.698	0.892	0.718
	10	0.606	0.790	0.854

Table B.2 Regression analyses results using the script developed discarding validation data.

Training Function	Hidden Neuron #	MLVSS	Ss	Xhet
trainb	5	0.932	0.910	0.911
	6	0.928	0.881	0.958
	9	0.860	0.971	0.964
	10	0.987	0.928	0.950
trainbfg	3	0.985	0.993	943.000
	4	0.985	0.964	0.977
	5	0.992	0.988	0.998
	6	0.988	0.967	0.950
trainbfg	8	0.990	0.988	0.928
	10	0.986	0.965	0.978
trainbr	2	0.982	0.992	0.937
	3	0.988	0.992	0.946
	4	0.992	0.993	0.982
	5	0.992	0.994	0.980
	6	0.993	0.994	0.992
	7	0.991	0.994	0.991
	8	0.996	0.990	0.995
	9	0.996	0.991	0.994
	10	0.995	0.994	0.990
traincgb	4	0.973	0.954	0.947
	5	0.986	0.973	0.977
	7	0.992	0.991	0.963
	8	0.989	0.972	0.997
	9	0.980	0.966	0.994
	10	0.998	0.987	0.995
traincgf	3	0.985	0.993	0.943
	4	0.985	0.993	0.943
	5	0.992	0.976	0.993

Table B.2 (Continued).

traincgf	6	0.996	0.988	0.994
	7	0.992	0.978	0.957
	8	0.987	0.992	0.979
traincgf	10	0.983	0.981	0.994
traincgp	3	0.985	0.993	0.943
	4	0.990	0.998	0.998
	5	0.993	0.986	0.900
	6	0.989	0.975	0.998
	7	0.996	0.979	0.994
	8	0.983	0.990	0.984
	9	0.988	0.967	0.990
	10	0.997	0.984	0.999
traingd	1	0.984	0.751	0.966
traingda	2	0.983	0.992	0.932
	3	0.985	0.993	0.942
	4	0.985	0.993	0.941
	5	0.993	0.991	0.964
	6	0.996	0.988	0.991
	7	0.993	0.984	0.973
traingda	8	0.994	0.986	0.985
	9	0.988	0.992	0.992
	10	0.998	0.993	0.992
traingdm	-	-	-	-
traingdx	3	0.985	0.993	0.943
	4	0.989	0.992	0.948
	5	0.982	0.987	0.989
	6	0.993	0.984	0.999
	7	0.987	0.980	0.965
	8	0.995	0.982	0.995
	9	0.993	0.977	0.989
	10	0.994	0.982	0.987
trainlm	2	0.982	0.992	0.941
	3	0.991	0.989	0.921
	5	0.987	0.966	0.985
	6	0.994	0.979	0.985
trainoss	2	0.985	0.993	0.943
	3	0.995	0.995	0.961
	4	0.993	0.989	0.910

Table B.2 (Continued).

trainoss	5	0.994	0.992	0.972
	6	0.996	0.987	0.995
	7	0.991	0.978	0.963
	8	0.980	0.968	0.994
	10	0.988	0.972	0.910
trainrp	3	0.993	0.989	0.910
	4	0.996	0.986	0.964
	5	0.998	0.995	0.960
	6	0.997	0.984	0.793
	7	0.993	0.972	0.965
	8	0.992	0.982	0.994
	9	0.994	0.985	0.992
	10	0.994	0.987	0.986
trainscg	3	0.984	0.993	0.942
	4	0.981	0.974	0.987
	5	0.993	0.981	0.996
	6	0.988	0.988	0.951
	7	0.987	0.966	0.998
	8	0.988	0.966	0.994

APPENDIX C

Results of runs with IskWTP Data

Table C.1. Complete results of IskWTP run NO:25.

training function	Set	HNs	R
trainbfg	5	5	0.622
trainbfg	6	3	0.620
trainbfg	6	4	0.673
trainbfg	6	6	0.640
traincgb	5	3	0.603
traincgb	5	6	0.795
traincgb	6	4	0.616
traincgb	6	6	0.694
traincgf	5	4	0.648
traincgf	6	6	0.649
traincgp	5	5	0.664
traincgp	6	2	0.653
traingd	6	4	0.639
trainlm	6	1	0.670
trainoss	5	3	0.628
trainscg	6	6	0.668

Table C.2. Complete results of IskWTP run NO:26.

training function	Set	HNs	R
trainb	4	2	0.696
trainb	4	6	0.658
trainbfg	4	3	0.650
trainbfg	4	5	0.648
trainbfg	5	3	0.673
trainbfg	5	5	0.653
trainbfg	5	6	0.673

Table C.2. (continued).

trainbr	2	7	0.627
trainbr	4	3	0.654
trainbr	4	7	0.639
trainbr	5	3	0.691
trainbr	6	3	0.633
traincgb	5	6	0.615
traincgp	4	4	0.627
traincgp	5	2	0.693
traingd	4	7	0.628
traingd	5	4	0.612
trainga	6	7	0.615
traingdm	4	2	0.627
traingdm	4	3	0.656
traingdm	4	5	0.661
trainlm	4	4	0.729
trainlm	4	6	0.709
trainlm	4	7	0.684
trainlm	6	5	0.646
trainoss	4	2	0.650
trainoss	4	5	0.646
trainoss	4	6	0.638
trainoss	5	1	0.652
trainrp	4	1	0.650
trainrp	5	4	0.703
trainscg	4	2	0.634
trainscg	4	4	0.669

APPENDIX D
CODES & SCRIPTS WRITTEN

D.1. MATLAB Script Written for Automated Generation ANN Models

```
echo off
fortr={'b'  ;'bfg';'br' ;'cgb';'cgf';'cgp';'gd' ;'gda';'gdm';'gdx';'lm' ;'oss';'rp' ;'scg'};
trspaces={'  ';"   ;' ' ;"   ;"   ;"   ;' ' ;"   ;"   ;"   ;' ' ;"   ;' ' ;"   };
[numf1 numf2]=size(fortr);
tn=(norm01(TarAll))';
r=0;
for all=6:6 %input kombo sayisi
   pn = eval(char(strcat(['(norm01(Orginp'],[num2str(all,'%02d')],['))";'])));
   [R,Q] = size(pn);
   iitr = 1:floor(Q*0.50);
   iival = ceil(Q*0.50):floor(0.75*Q);
   iitst = ceil(0.75*Q):1:Q;
   validation.P = pn(:,iival);
   validation.T = tn(:,iival);
   testing.P = pn(:,iitst);
   testing.T = tn(:,iitst);
   ptr = pn(:,iitr);
   ttr = tn(:,iitr);
   for y= 1:numf1
        DizinYarat(y)=strcat(['mkdir(…
        .\nettrain'],[fortr(y)],['_'],strcat([num2str(all,'%02d')]),[trspaces(y)],[';']);
        DizinYaratti(y,:)=char(DizinYarat(y));
        eval(DizinYaratti(y,:));
   end
```

```
   for j= 1:numf1 %changing the training function
      for i=1:6 % changing number of hidden neurons in the net...
            cd('E:\iskenderun0dan\ilkdeneme\memory'); % hafizayi toparliyor...
            pack;
            cd('E:\iskenderun0dan\ilkdeneme');
NetOlustur(i)=strcat(['nettrain'],[fortr(j)],[num2str(i,'%02d')],['_'],…
strcat([num2str(all,'%02d')]),[ '=newff(minmax(ptr),['],num2str(i,'%02d'),['…
'],num2str(i,'%02d'),[ ' 1],{"logsig","logsig","logsig"},"train"],[fortr(j)],[""');'],…
[trspaces(j,:)],[trspaces(j,:)]);
          NetOlusturdu(i,:)=char(NetOlustur(i));
          eval(NetOlusturdu(i,:));
          NetAyarla1(i)=strcat(['nettrain'],[fortr(j)], num2str(i,'%02d')…
          ,['_'],strcat([num2str(all,'%02d')]), ['.trainParam.epochs=20000;',...
          'nettrain'],[fortr(j)], num2str(i,'%02d'),['_'],strcat([num2str(all,… '%02d')]),
          ['.trainParam.goal=0.000;'],[trspaces(j,:)],[trspaces(j,:)]);
          NetAyarlandi1(i,:)=char(NetAyarla1(i));
          eval(NetAyarlandi1(i,:));
          if strcmp(fortr(j),'bfg')
                NetAyarla1a(i)=strcat(['nettrain'],[fortr(j)],…
                num2str(i,'%02d'),['_'],strcat([num2str(all,'%02d')]),...
                ['.trainParam.searchFcn="srchcha";'],[trspaces(j,:)]);
                NetAyarlandi1a(i,:)=char(NetAyarla1a(i));
                eval(NetAyarlandi1a(i,:));
           end
          Egit(i)=strcat( ['[nettrain'],[fortr(j)],[num2str(i,'%02d')],['_'],…
          strcat([num2str(all,'%02d')]),[',trres'],[fortr(j)],...
          [num2str(i,'%02d')],['_'],strcat([num2str(all,'%02d')]),[ …
          ']=train(nettrain'],[fortr(j)], [num2str(i,'%02d')],['_'],...
          strcat([num2str(all,'%02d')]),[',ptr,ttr,[],[],validation,testing);…
          clf;close(gcf);'],[trspaces(j,:)],[trspaces(j,:)],[trspaces(j,:)]);
          Egitti(i,:)=char(Egit(i));
```

```
eval(Egitti(i,:));
Dene(i)=strcat(['[restrain'],[fortr(j)], num2str(i,'%02d'),['_'], …
strcat([num2str(all,'%02d')]), [']'],['=sim(nettrain' ],[fortr(j)], ...
num2str(i,'%02d'),['_'],strcat([num2str(all,'%02d')]),…
[',pn);'],['Prestrain'],[fortr(j)], num2str(i,'%02d'),['_'],...
strcat([num2str(all,'%02d')]),['= unnorm01(TarAll …
'],[',restrain'],[fortr(j)],[num2str(i,'%02d')],['_'],...
strcat([num2str(all,'%02d')]),[');'],[trspaces(j,:)],…
[trspaces(j,:)],[trspaces(j,:)],[trspaces(j,:)]);
Denedi(i,:)=char(Dene(i));
eval(Denedi(i,:));
HesaplaCizdir3(i)=strcat(['fig'],[fortr(j)], [num2str(i,'%02d')],…
['_'],strcat([num2str(all,'%02d')]),['Reg=figure;'],...
['[m'],[fortr(j)],num2str(i,'%02d'), [',b'],[fortr(j)], …
num2str(i,'%02d'),[',r'],[fortr(j)],num2str(i,'%02d'),...
[']=postreg(Prestrain'],[fortr(j)], num2str(i,'%02d'),['_'],…
strcat([num2str(all,'%02d')]),['",TarAll'],[');'],…
['title("Regression analysis for (train'],fortr(j),['_'],…
strcat([num2str(all,'%02d')]),[')'],['(#of HNs:'],[num2str(i,'%02d')],…
[') ");'],trspaces(j),trspaces(j),trspaces(j),trspaces(j),trspaces(j),trspaces(j));
Hesapladi3(i,:)=char(HesaplaCizdir3(i));
eval(Hesapladi3(i,:));
regresValue=eval(char(strcat(['r'],[fortr(j)],num2str(i,'%02d'))));
if regresValue>=0.40
   Kaydet3(i)=strcat(['print("-r300","-djpeg",".\nettrain'],
         [fortr(j)],['_'],strcat([num2str(all,'%02d')]),...
         ['\fig'],[fortr(j)],num2str(i,'%02d'),['Reg"' '
         );'],['close(gcf);'],trspaces(j),trspaces(j));
Kaydetti3(i,:)=char(Kaydet3(i));
eval(Kaydetti3(i,:));
HesaplaCizdir1(i)=strcat(['fig'],[fortr(j)], num2str(i,'%02d'),…
```

```
        ['_'],strcat([num2str(all,'%02d')]),['=figure; plot(trres'],…
        [fortr(j)], num2str(i,'%02d'), ['_'],strcat([num2str(all,'%02d')]),...
        ['.epoch,trres'], [fortr(j)], num2str(i,'%02d'), ['_'],…
        strcat([num2str(all,'%02d')]), ['.perf,"r", trres'],[fortr(j)],…
        num2str(i,'%02d'),['_'],strcat([num2str(all,'%02d')]), ...
        ['.epoch,trres'], [fortr(j)], num2str(i,'%02d'), ['_'],…
        strcat([num2str(all,'%02d')]),['.vperf,":g",trres'],[fortr(j)],…
        num2str(i,'%02d'),['_'],strcat([num2str(all,'%02d')]),...
        ['.epoch,trres'], [fortr(j)], num2str(i,'%02d'),…
        ['_'],strcat([num2str(all,'%02d')]),...
        ['.tperf,"-.b");'],['xlabel("# of epoch");'],...
        [trspaces(j,:)],[trspaces(j,:)],[trspaces(j,:)],[trspaces(j,:)],…
        [trspaces(j,:)],[trspaces(j,:)],[trspaces(j,:)]);
Hesapladi1(i,:)=char(HesaplaCizdir1(i));
eval(Hesapladi1(i,:));
HesaplaCizdir11(i)=strcat(['title("MSE vs # of Epochs (train'] ,…
        [fortr(j)],['_'],strcat([num2str(all,'%02d')]),...
        [')'],[' (# of HNs:'],num2str(i,'%02d'),[')");'],[trspaces(j)],…
        ['legend("training","Validation","Test",0);…
        ylabel("Mean Squared Error");']);
Hesapladi11(i,:)=char(HesaplaCizdir11(i));
eval(Hesapladi11(i,:));
Kaydet1(i)=strcat(['print("-r300","-djpeg",".\nettrain'],…
        [fortr(j)],['_'],strcat([num2str(all,'%02d')]),['\fig'],[fortr(j)], ...
        num2str(i,'%02d'),['_'],strcat([num2str(all,'%02d')]),['");…
        close(gcf);'],[trspaces(j,:)],[trspaces(j,:)]);
Kaydetti1(i,:)=char(Kaydet1(i));
eval(Kaydetti1(i,:));
HesaplaCizdir2(i)=strcat(['fig'],[fortr(j)], num2str(i,'%02d'),…
        ['OwP'], ['=figure; plot(DATE,Prestrain'],[fortr(j)],...
```

```
            num2str(i,'%02d'),['_'],strcat([num2str(all,'%02d')]),['.-r"…
            '],[',DATE,TarAll,"-b");'],...
            ['legend("Predicted","Observed",0); '],['ylabel("COD_{eff}…
            (mg/l)");'],['xlabel("Date");'],...
            ['title("Pred & Obs COD_{eff} (mg/l) vs Date w/ train '], …
            [fortr(j)],['_'],strcat([num2str(all,'%02d')]), ['(# of HNs:',…
            num2str(i,'%02d'),')");'],[trspaces(j)],[trspaces(j)],[trspaces(j)]);
        Hesapladi2(i,:)=char(HesaplaCizdir2(i));
        eval(Hesapladi2(i,:));
        Kaydet2(i)=strcat(['print("-r300","-djpeg",".\nettrain'],…
            [fortr(j)],['_'],strcat([num2str(all,'%02d')]),['\fig'],…
            [fortr(j)], num2str(i,'%02d'),['OwP"' '); close(gcf);'],…
            [trspaces(j)],[trspaces(j)]);
        Kaydetti2(i,:)=char(Kaydet2(i));
        eval(Kaydetti2(i,:));
      end
    Kaydet4(i)=strcat([ 'save .\nettrain'],[fortr(j)] ,['_'],…
            strcat([num2str(all,'%02d')]), ['\nettrain'],[fortr(j)],…
            num2str(i,'%02d'),['_'],strcat([num2str(all,'%02d')]),… [' net* …
            Prestrain* restrain* trres*'],[' m'],fortr(j),['*'],[' b'],fortr(j),...
            ['* r'],fortr(j),['*'],[';close(gcf);'],['clear net* Prestrain* restrain*…
             trres* fig* m'],fortr(j),['* b'],fortr(j), ['* r'],fortr(j),['*'],…
            trspaces(j),trspaces(j),trspaces(j),trspaces(j),…
            trspaces(j),trspaces(j),trspaces(j),trspaces(j));
    Kaydetti4(i,:)=char(Kaydet4(i));
    eval(Kaydetti4(i,:));
    cd('E:\iskenderun0dan\ilkdeneme\memory');
    pack;
    cd('E:\iskenderun0dan\ilkdeneme');
  end
end   end
```

D.2. C Code that divides ACWTP data into three equal pieces using PGAPack Genetic Algorithm Library.

```
#include <stdio.h>
#include <stdlib.h>
#include "/usr/local/pga/include/pgapack.h"
#define DataLength 96

double evaluate(PGAContext *,int  , int );
float realdata[DataLength];
float theone=0;
float datasorted[DataLength];
FILE *dosya;

int main(int argc, char **argv)
{
 int u;
 dosya=fopen("ank96sort.txt","r");
 for (u=0;u<DataLength;u++)
 {
  fscanf(dosya,"%f",&(realdata[u]));
  //printf("deger %d : %f\n ",u,realdata[u]);
  theone=theone+realdata[u];
 }
 theone=(float) theone/DataLength;
 PGAContext *ctx;
 ctx=PGACreate(&argc,argv,PGA_DATATYPE_BINARY,
        DataLength,PGA_MINIMIZE);
 PGASetStoppingRuleType(ctx,PGA_STOP_NOCHANGE);
 PGASetUp(ctx);
 PGARun(ctx, evaluate);
```

```
  PGADestroy(ctx);
  dosya=fopen("result.txt","w");
  for (u=0;u<DataLength;u++)
          fprintf(dosya,"%f\n",datasorted[u]);
  fclose(dosya);
  return EXIT_SUCCESS;
}
double  evaluate(PGAContext *ctx,int p, int pop)
{
  int i,j=0,k=0,t=0;
  int stringlen;
  float  data1=0.0f,data2=0.0f,data3=0.0f;
  for(i=0;i<DataLength;i++)   //sort the array
  {
   if(PGAGetBinaryAllele(ctx,p,pop,i))
   {      datasorted[j]=realdata[i];
          j++;    }
   else
   {      datasorted[DataLength-k-1]=realdata[i];
          k++;    }
  }
   for (i=0;i<DataLength;i++)
   {
    if(i<(DataLength/3))
      data1=data1+datasorted[i];
    else if (i>=(DataLength/3) && (i<(2*DataLength/3)))
      data2=data2+datasorted[i];
    else if (i>=(2*DataLength/3))
      data3=data3+datasorted[i];
   }
    data1=(float) (data1/((float)(DataLength/3)));
```

```
    data2=(float) (data2/((float)(DataLength/3)));
    data3=(float) (data3/((float)(DataLength/3)));
        //printf("difference : %f \n",(double)(pow(theone-data1,2)+pow(theone-
        // data2,2)+pow(theone-data3,2)));
    return (double) (pow(theone-data1,2)+pow(theone-data2,2)+pow(theone-
    data3,2));
}
```