Chapter 2

Literature Review

In this chapter a review of the applications of neural networks in chemical engineering especially in process control is provided. Their applications varied in a wide range from their use in advanced process controls, such as predictive control, inverse-model-based control, and adaptive control. Neural networks are also utilized in other applications: online estimation, pattern recognition, data rectification, gross error detection, etc. Some papers (Thibault and Grandjean, 1991; Willis et al., 1991; Willis et al., 1992, and Hussain, 1999) reviewing the use of neural networks in control applications, and some books (Miller, Sutton, and Werbos, 1990; Bulsari, 1995) describing the use of neural networks in control of various processes, are available.

This chapter is divided into four sections: types of artificial neural networks, chemical process modeling and identification with neural networks, neural networks in advanced control, and other applications of neural networks in chemical engineering as follows.

2.1 Types of Artificial Neural Networks

The number of different types of artificial neural network architectures and node processing functions that are available in the literature is large (Morris, Montague, and Willis, 1994). The selection of the neural network depends on the purpose of their applications. However those that are commonly found in engineering applications are the multilayer feedforward networks, recurrent networks and radial basis function networks. The multilayer feedforward network with one hidden layer structure is depicted in Figure 2.1. The description of multilayer feedforward networks will be given in detail in the next chapter.

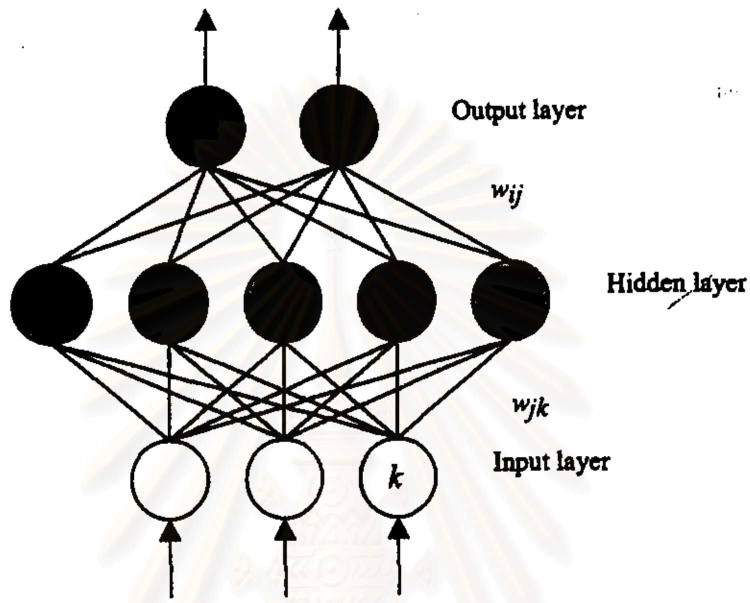

Figure 2.1: Multilayer feedforward network architecture with one hidden layer.

The architecture of recurrent networks as shown in Figure 2.2 is quite similar to that of the multilayer feedforward networks except that there are also feedback and lateral connections between the nodes in the same as well as in the different layers. Networks that have feedback only from the output layer are called external recurrent networks, while those that have feedback to and/or from the hidden layer are called internal recurrent networks (Su and McAvoy, 1992).

The radial basis function networks are also similar to the multilayer feedforward networks with some exceptions. One is that the activation function is in terms of some radial basis function such as the Gaussian or spline function (Brown and Harris, 1994). Secondly, there is no nonlinear activation function at the output layer (i.e. linear output) and hence the weights between the hidden and output layer can be determined by linear regression techniques (Chen and Billings , 1992). Radial basis function network structure is illustrated in Figure 2.3.

Nevertheless the multilayer feedforward network with sigmoid or hyperbolic tangent activation function is by far the most widely applied. It is also global in representation and normally requires smaller number of hidden nodes as compared to the radial basis function networks (Boslovic and Narendra, 1995; Edward and Goh, 1995). The multilayer feedforward network with sigmoid or hyperbolic tangent activation function is also computationally less intensive (during training) compared to the recurrent-type networks. A number of neural network learning strategies have been developed elsewhere (Rumelhart and McClelland, 1986; Lippmann, 1987).

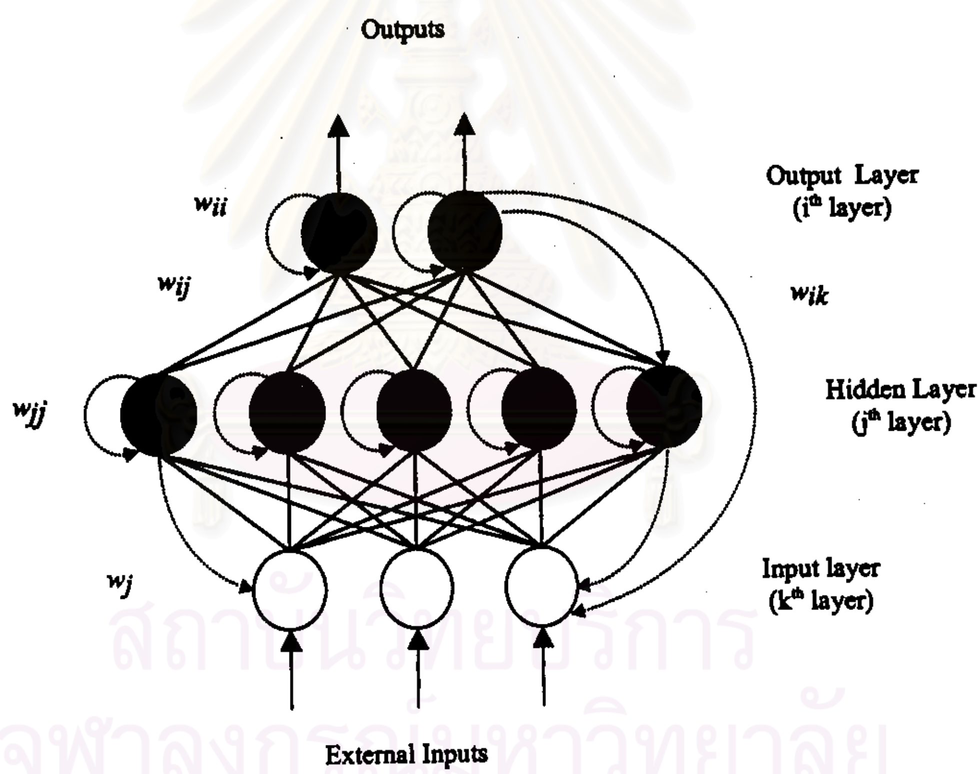

Figure 2.2: Recurrent neural network architecture.

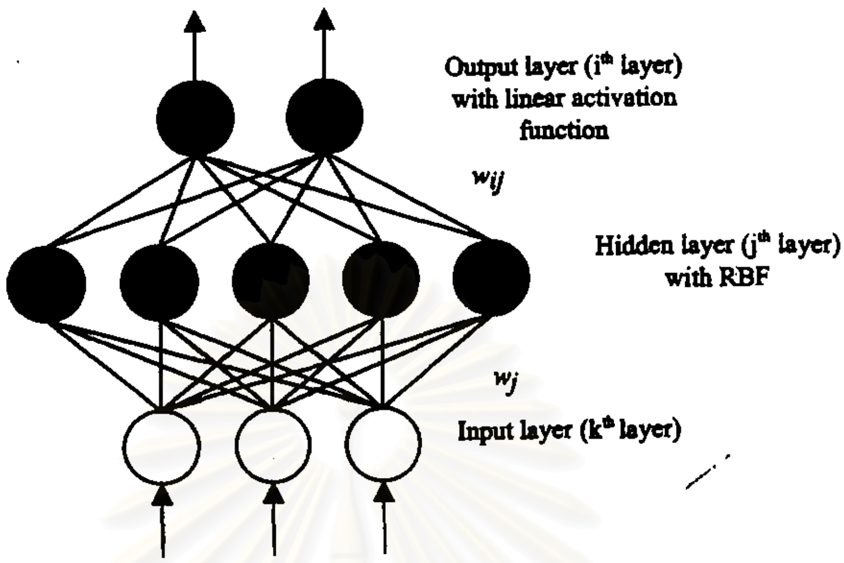

Figure 2.3: Radial basis function network architecture.

2.2 Chemical Process Modeling and Identification with Neural Networks

Many systems of interest in chemical engineering are highly nonlinear. The often-complicated dynamic behavior of such system can be successfully analyzed, characterized and predicted using neural networks to construct black-box models (empirical models) and gray-box models (semi-empirical models). These models can be used for the control and/or optimization of the processes. In this section the use of neural networks for the purpose of modeling and identification is proposed.

2.2.1 Black-box Modeling Approach

Neural networks as black-box modeling tools have already been used for many applications in industry, business, and science (Widrow et al., 1994). The ability of neural networks to approximate any continuous function to any desired of accuracy (Cybenko, 1989) has been the basis for many applications. Nonetheless, only their applications in chemical engineering are headings presented. Multilayer feedforward networks, recurrent neural networks, and radial basis function networks are mostly utilized in chemical engineering especially for the purpose of system modeling and/or identification. According to the review on neural network application in chemical process modeling, either simulated data or real plant data are used to identify the process models.

Multilayer Feedforward Networks (MFFNs)

Many researches employed this network topology as a black-box modeling tool to model many systems either simulation or online. In accordance with the simulation applications, the MFFNs were utilized to model many processes: continuous stirred tank reactors, pH neutralization processes, biochemical processes, distillation, catalytic process, desalination, vapor composition and some linear/nonlinear systems. The abbreviations used in this chapter is given in Table 2.1 and the neural network applications to simulated and real processes are summarized in Table 2.2 and Table 2.3, respectively.

An application to steady state reactor modeling was given by Bhat and McAvoy (1989, 1990), in which an isothermal CSTR reactor is considered and a MFFN was trained to optimize the reactor yield. Bhat and McAvoy (1989, 1990) and Saint-Donat, Bhat, and McAvoy (1991) used a MFFN for the dynamic modeling of a simulated nonlinear pH system. Narendra and Parthasarathy (1990) introduced the models that MFFN and recurrent neural network (RNN) were interconnected in novel configuration for both identification and control. It was found that the neural networks could be used effectively for the identification and control of nonlinear dynamical systems. Nahas, Henson, and Seborg (1992) utilized the three-layer feedforward networks trained with a conjugated gradient algorithm to model the continuous stirred tank reactor (CSTR) and the pH neutralization process and implement them in the nonlinear internal model control (NIMC). Nikravesh, Farell, and Standford (1996) adopted the MFFN in conjunction with recursive least squares to identify the model of a nonisothermal CSTR with time varying parameters. They found that their technique could be used effectively for model identification of nonlinear time variant processes.

Ungar, Powell, and Kamens (1990) modeled a bioreactor with two controlled variables and one manipulated variable using MFFN. Kurtanjek (1994) studied the use of MFFN to model the baker 's yeast production. Ribiera-Polak with Powell modification algorithm was adopted to train the network. This study found that the network was effective tool for modeling of complex system such as biological processes. Piron, Latrille, and René (1997) applied the MFFN in black-box modeling and gray-box (semi-physical or hybrid) modeling to the study of the crossflow microfiltration process which was performed on suspensions of baker 's yeast. It was found that the hybrid approach appeared to be more accurate and was a means for complementing the description of a physical model. They also concluded that further applications (especially controls), however, remain restricted by the assumption made to establish this model. Classical networks ("black-box" approach) certainly do not have this limitation for process understanding. Emmanouilides and Petrou (1997) used the MFFN to identify and control an anaerobic digester process. Adaptive online training with random search optimization techniques, random search and chemotaxis, as well as backpropagation algorithm were applied to improve the modeling and control performance. From the results, the random search techniques converged much faster than the backpropagation algorithm.

Lambert and Hecht-Nielson (1991) compared MFFN and fully recurrent networks for the prediction of the molar fraction in the bottom stream of a binary distillation. MacMurray and Himmelblau (1995) examined a number of different types of artificial neural networks, including MFFN, externally recurrent network (ERN), internally recurrent (Elman) network (IRN), diagonally recurrent network (DRN), and combinations of ERN and IRN, to model the packed distillation column. They found that externally recurrent network (ERN) had the best performance in predicting the process output many time step ahead in the future, furthermore, the network model was as good or better than a simplified first principles model when used for model predictive control.

Chitra (1992) described an application of MFFN for developing chemical kinetics of a catalytic process. The neural network model was better in several temperature and catalytic loading regions, compared to a statistical power-law model and quadratic model.

Ramasamy and Deshpande (1995) investigated the application of MFFN in process identification as demonstrated a simulated multistage desalination process. They stated that feedforward network offer a great potential for applications in process identification and advanced control.

Fakhr-Eddine et al. (1996) utilized an alternative approach to Low Pressure Chemical Vapor Decomposition (LPCVD) modeling. That is the reactor was broken up into a number of basic elements in which a MFFN was elaborated to represent. The network, trained with quasi-Newton learning algorithm, was used to compute on-line the film thickness on each wafer in order to develop a controller of LPCVD reactors then good model was obtained. Nevertheless, they concluded that the computation rapidity of the neural network model which enables its use in control aim as on-line sensors of film thickness are not available.

Lou and Perez (1996) used the backpropagation algorithm in conjunction with Kalman filtering in order to establish a new self-learning technique of MFFN. They found that this new technique was faster and more stable than the classical backpropagation algorithm for training MFFN. Moreover, it was less sensitive to the initial weights and to the learning parameters.

Some researches were also utilized the MFFN to model real processes. Pollard et al. (1992) demonstrated that MFFN models could be built for real industrial processes. They conducted experiments on a distillation column unit with one input (column reflux flow rate) and one output (tray temperature) and obtained a neural network dynamic model. They also demonstrated the utility of cross validation. Baratti, Vacca, and Servido (1995) utilized the MFFN to model the two actual distillation columns: the butane splitter tower and the gasoline stabilizer and then implemented them for monitoring and control applications. They found that neural network model with proper implementation techniques can significantly improve column operation.

Blum et al. (1992) and Blum (1992) used a MFFN to model a multiple-input multiple-output (MIMO) reactor in the Tennessee Eastman plant (Downs and Vogel, 1993).

Ramasamy and Deshpande (1995) investigated the application of MFFN in process identification as demonstrated an industrial multivariable process. They stated that MFFNs offer a great potential for applications in process identification and advanced control.

Recurrent Neural Networks (RNNs)

Regarding the research works that are surveyed, there are few papers applied recurrent neural network for modeling. One employed the network to model the neutralization in continuous stirred tank reactor, the other investigated its use in linear and nonlinear systems.

You and Nikolaou (1993) utilized the recurrent neural network (RNN) to model both static and dynamic relationship of a pH CSTR and a biochemical batch reactor. They found that the modeling capabilities of RNN were comparable to those of the MFFN, but the training of RNN took longer time. Pham and Liu (1993) investigated the use of the basic Elman-type recurrent network and the modified Elman network, in which self-connections are made to the context units for the identification of a variety of linear aud nonlinear systems. It was found that the latter networks were more versatile than the basic Elman nets in being able to model the dynamic behavior of high order linear and nonlinear systems.

Radial Basis Function Networks (RBFNs)

Chen and Billings (1992) and several others have also studied neural networks for system identification, obtaining Nonlinear Auto-Regressive Moving Average with eXogenous inputs (NARMAX) type models. Pottmann and Seborg (1997) showed how RBFN could be used to predict pH in a CSTR.

2.2.2 Gray-box Modeling Approach

Despite the use of the neural networks as the black-box modeling tools, there have been recent attempts to apply the neural networks in gray-box type modeling. In this approach, the neural networks are used to estimate the parameters and unmeasured states of the first principle model therefore sometimes the models obtained are called hybrid models. Multilayer feedforward network and radial basis function network were utilized in these researches. The summary of the neural network application to chemical processes with gray-box approach is provided in Table 2.4.

Multilayer Feedforward Networks (MFFNs)

Psichogios and Ungar (1992) developed a hybrid model for a fedbatch bioreactor. The hybrid model combined a partial first principles model, which incorporated the available prior knowledge about the process being model, with a neural network which served as an estimator of unmeasured process parameters that are difficult to model from first principles. The training method for the neural network was the error backpropagation algorithm. They found that the hybrid model had better properties than standard black-box neural network model in that it is able to interpolate and extrapolate much more accurately. Furthermore, it was easier to analyze and interpret and required significantly fewer training examples.

In addition to the simulation applications, MFFNs were also applied to identify real processes. Henricus et al. (1996) utilized serial gray-box modeling for dynamic modeling of real-time pressure vessel. Noniterative training algorithm, which is very fast, was used for training the neural networks. In this strategy, a neural network was used to model the inaccurately known term of a macroscopic balance, and the identification data covered only the input-output space of the inaccurately known term. They stated that the serial gray-box configuration resulted in accurate models with known extrapolation properties with a limited experimental effort.

Sabharwal, Bhat, and Wada (1997) used the approach that integrated a neural network and dynamic simulation modeling to achieve quality control and increase throughput. It was developed for the no. 2 XY splitter of the xylene distillation unit as part of a new advanced quality control (AQC) project in the Japan Energy Corp. Mizushima Oil Refinery.

Radial Basis Function Networks (RBFNs)

Semi-parametric approaches combining radial basis function network (RBFN), serving as an estimator of unmeasured process parameters, with prior models either in series or parallel have been studied by Thompson and Kramer (1994). The RBFN weights were estimated using nonlinear programming methods. The inclusion of the prior knowledge was investigated as a means of improving the neural network predictions when they were trained in sparse and noisy process data. The approach was applied in predicting cell biomass and secondary metabolite in a fed-batch penicillin fermentation. They showed that the prior knowledge enhanced the generalization capabilities of a neural model.

Table 2.1: Description of abbreviations

Abbreviations	Description
Neural network type	
DRN	Diagonally Recurrent Network
ERN	External Recurrent Network
IRN	Internal Recurrent Network
MFFN	Multilayer FeedForward Network
RBFN	Radial Basis Function Network
RNN	Recurrent Neural Network
Activation/ Transfer Function	
Ellp	Ellipse
Lin	Linear
RBF	Radial Basis Function
Sig	Sigmoid Function
Tanh	Hyperbolic Tangent Function
System/Objective	
Bio	Bioprocess/ Bioreactor
CSTR	Continuous Stirred Tank Reactor
Dis	Distillation
Neut	Neutralizing/ Neutralizer
Comp	Composition
Conc	Concentration
MW	Molecular Weight
Poly	Polymerization
Press	Pressure
Prod	Product
Temp	Temperature
Thick	Thickness
Control technique	
DMC	Dynamic Matrix Control
GMC	Generic Model Control
IMC	Internal Model Control
MPC	Model Predictive Control
PI	Proportional Integral
PID	Proportional Integral Derivative
Robustness	
Dist	Disturbance Rejection
Set pt	Set point Tracking

Table 2.2: Neural network applications in simulated process modeling with black-box approach

NN type	Training algorithm	System	References
MFFN/Sig	backpropagation	CSTR	Bhat and McAvoy, 1989; 1990
MFFN/Sig	backpropagation	pH system	Bhat and McAvoy, 1989, 1990; Saint-Donat et al., 1991
MFFN/RNN	backpropagation	nonlinear system	Narendra and Parthasarathy, 1990
MFFN	backpropagation	Bioreactor	Ungar et al., 1990
MFFN/RNN	backpropagation	binary distillation	Lambert and Hecht-Nielson, 1991
MFFN/Sig	conjugate gradient	CSTR/ pH system	Nahas, Henson, and Seborg, 1992
MFFN	backpropagation	catalytic process	Chitra, 1992
MFFN/Tanh	recursive least square	CSTR	Nikravesh, Farell, Standford, 1996
MFFN	Ribiera-Polak with Powell modification	yeast production	Kurtanjek, 1994
MFFN/ERN/ DRN/ERN+IRN	backpropagation	packed dis. column	MacMurray and Himmelblau, 1995
MFFN/Sig	backpropagation	desalination	Ramasamy and Deshpande, 1995
MFFN/Sig	quasi-Newton	LPCVD	Fakhr-Eddine et al., 1996
MFFN/Tanh	backpropagation with kalman filtering	nonlinear system	Lou and Perez, 1996
MFFN/Sig	quasi-Newton	cross flow microfiltration	Piron, Latrille, and René, 1997
MFFN	random search opt tech, random search, chemotaxis, and backpropagation	anaerobic digestion	Emmanouilides and Petrou, 1997

Table 2.3: Neural network applications in real process modeling with black-box approach

NN type	Training algorithm	System	References
MFFN/Sig	backpropagation	distillation	Pollard et al., 1992
MFFN	backpropagation	MIMO reactor	Blum et al., 1992; Blum, 1992
RBFN	backpropagation	pH system	Chen and Billings, 1992
RBFN	backpropagation	pH system	Pottmann and Seborg, 1992
RNN/Sig	back propagation through time	pH system and Bio.	You and Nikolaou, 1993
RNN/Lin, Sig, Tanh	backpropagation	linear/ nonlinear system	Pham and Liu, 1993
MFFN/Sig	backpropagation	multivariable process	Ramasamy and Deshpande, 1995
MFFN	backpropagation	splitter tower and gasoline stabilizer	Baratti, Vacca, and Servido, 1995

Table 2.4: Neural network applications in chemical modeling with gray-box approach

NN type	Training algorithm	System	References
MFFN	backpropagation	fedbatch bioreactor	Psichogios and Ungar, 1992
RBFN	backpropagation	fedbatch penicillin fermentation	Thompson and Kramer, 1994
MFFN/Tanh	noniterative training	pressure vessel	Henricus et al., 1996
MFFN	backpropagation	splitter of xylene distillation	Sabharwal, Bhat, and Wada, 1997

2.3 Neural Network Applications in Control Systems

The majority of the neural networks utilized in these applications are multilayer feedforward networks, recurrent networks, and radial basis function networks. There is no clear advantage of one network over the other as well as of one activation function over the other. This will very much be dependent on the user and their application and has to be looked on a case-to-case basis. Some comparisons between the different types of networks can be found in the research works of Karim and Rivera (1992) and Su and McAvoy (1992). While the comparisons between the conventional sigmoid and the radial basis function activation functions can be found in the research works of Weigand, Rumelhart, and Huberman (1990); Chen et al. (1990); and Edward and Goh (1995).

The applications utilizing these neural-network-based strategies are wide ranging but involve typical chemical process systems ranging from the linear to the highly nonlinear systems. The detailed description and characteristics of these processes can be found in standard textbooks (Douglas, 1972; Luyben, 1973; Perry, 1974; Stephanopoulos, 1984; and Seborg, Edgar, and Mellichamp, 1989). However, the most common systems used are the distillation columns and the reactor systems (continuous stirred tank reactors, bioreactors and the neutralizing reactors). These are multivariable, nonlinear systems, which are highly suitable for testing such control algorithms in chemical process systems. Neural networks are often used in many control configurations. However, those control systems can be grouped into three control techniques. That is model predictive control, inverse-model-based control, and adaptive control. The methodology to implement these control techniques, how neural networks are employed in the control configurations, and the neural network applications in those control configurations are proposed, respectively.

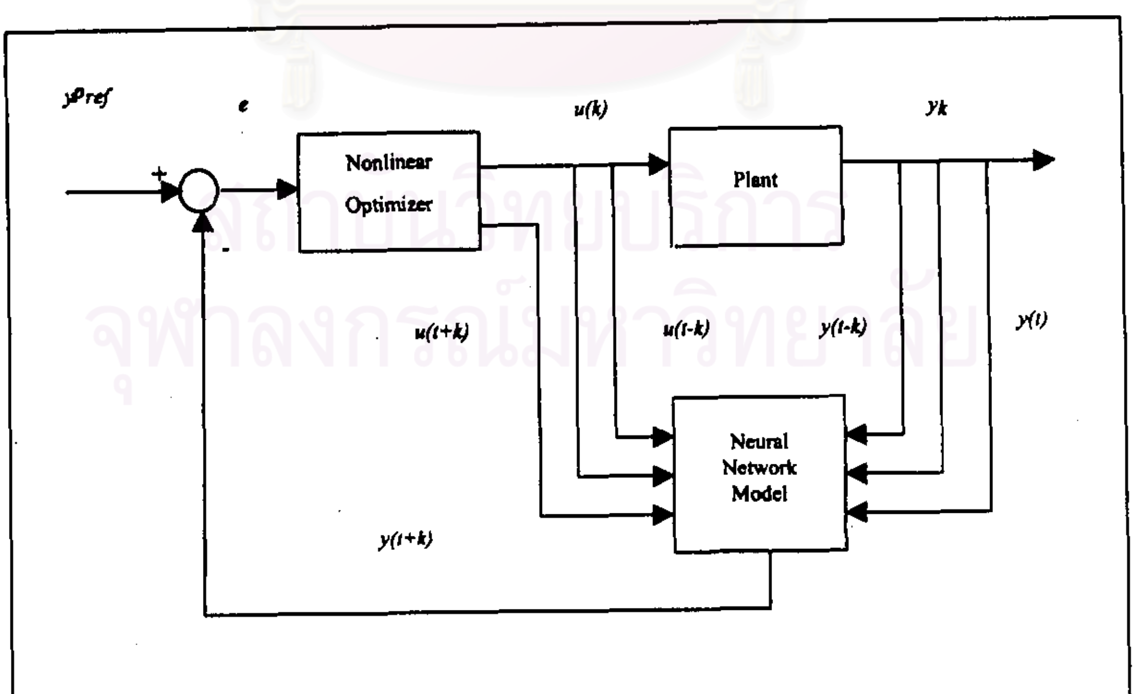

Figure 2.4: Neural networks in general model predictive control strategy.

2.3.1 Model Predictive Control Techniques

The most commonly found control technique, which uses neural network model is the predictive control technique. It is defined as a control scheme in which the controller determines a manipulated variable profile that optimize some open-loop performance objective on a time interval, from the current time up to a prediction horizon. Nonlinear model prediction control refers to the general case in which the model, performance objective and constraints are nonlinear functions of the system variables. In this case, neural networks are used as conventional identified models to replace the normal first-principle-models in the optimization formulation. The increasing popularity of the neural network-based-predictive technique is due to the attraction of using neural network models instead of other forms of model to effectively represent the complex nonlinear systems within the predictive methodology (Morris, Montague, and Willis, 1994). Some of the advantages of using neural networks in optimal control strategies over other conventional and linearly parameterized models are also given in the paper of Edward and Goh (1995).

Most of applications under the predictive control scheme utilize the multilayer feedforward neural network type while few utilize the recurrent type. These applications, with their objectives, systems and types of networks are summarized in Table 2.5 and Table 2.6. The major applications are described in further details later, beginning from the multilayer type.

Multilayer Feedforward Networks (MFFNs)

In one of the earliest reported simulation work, Psichogios and Ungar (1991) utilized a neural network model of a continuous stirred-tank reactor (CSTR) to control the product composition in the conventional model predictive scheme where they found that steady state offsets were obtained during set point tracking. However, they made corrections to the output, accounting for modeling error and unmeasured disturbances entering the process, and obtained offset-free tracking in this case. Willis, Montague, and Morris (1992) also estimated the plant-model mismatch at each sampling instant and utilized it to correct the predictions from the model in their model predictive control schemes. He implemented the control action using the receding horizon method, then implemented the scheme for the control of concentration in CSTR. Offset-free set point tracking results were obtained.

Two studies utilizing neural networks in the dynamic matrix control (DMC) algorithm have also been reported. Hernandez and Arkun (1990) applied neural networks to estimate the disturbance due to the presence of nonlinearities. This was then added to the linear model in the DMC formulation with online learning of the neural network models. This algorithm was applied for control of concentration in a CSTR system (with multiple steady states) for set-point tracking and disturbance-rejection case studies. They achieved better results in both cases as compared with the conventional linear DMC method. In the work of Lee and Park (1992) the neural network was taught to learn about the relationship between the disturbance pattern and the desired control actions by minimizing the controller output due to unmodeled effects. In this case the neural network basically acts as a feedforward controller to cater for unknown disturbances in the system. This scheme was then applied to control the compositions in the multiple reaction CSTR system under disturbances and plant-model mismatches. They found that the neural scheme performs better than the conventional feedforward DMC controller.

Hunt and Sbarbaro (1992) also estimated the plant-model mismatch at each sampling instant and utilized it to correct the predictions from the model in their model predictive control schemes. They implemented the control action using the receding horizon method then implemented it for the control of pH in a neutralizing reactor. Offset-free set point tracking results were obtained. Emmanouilides and Petrou (1997) utilized neural networks in a model predictive scheme to control the substrate concentration and pH of a complex nonlinear anaerobic digestion system. In his implementation, the neural network models were adapted online. The simulation results showed that the control strategy gave desired set point tracking and regulation even under process input variations and process parameter changes.

Turner, Montague, and Morris (1995) also estimated the plant-model mismatch at each sampling instant and utilized it to correct the predictions from the model in their model predictive control schemes. He implemented the control action using the receding horizon method then implemented it for the control of concentration in a distillation column. Offset-free set point tracking results were obtained. Lee and Park (1992) applied neural network in DMC configuration. The neural network was taught to learn about the relationship between the disturbance pattern and the desired control actions by minimizing the controller output due to unmodeled effects. In this case the neural network basically acts as a feedforward controller to cater for unknown disturbances in the system. This scheme was then applied to control the product compositions in a distillation column under disturbances and plant-model mismatches. They found that the neural scheme performs better than the conventional feedforward DMC controller. Gokhale, Horuwitz, and Riggs (1995) used a steady-state multilayer neural network model to replace the tray-to-tray model used in a predictive model based controller to control the product compositions in a propylene-propane splitter. They found that the neural-network scheme, with online filtering, performed slightly is better than the nonlinear model-based compositions (with sluggish response for the bottom composition).

For the applications to real processes, VanCan et al. (1995) utilized a neural network by numerically inverting the forward model and implementing it as a predictive controller. This was implemented on a laboratory pressure vessel to control the pressure by manipulating the inlet air flowrate. Experiments were done for set-point tracking and comparisons were made with the PI and linear model-based controllers. They found that the response of the neural network based controller was faster than the conventional approaches especially at larger set point changes.

Evans et al. (1993) developed a neural-network model of a laboratory process i.e. two non-interacting tanks in series, and incorporated it in a predictive control strategy, where the network was used to predict future process outputs up to a set horizon. Experiments for set point tracking of the level in the second tank were performed in this study. Their comparisons with the conventional PID controller show better performance, in terms of sluggishness and control movements.

Sheppard, Grant, and Ward (1992) applied neural networks for the control of temperature in a 175 kW experimental furnace system. In this case the neural network model was incorporated into an explicit generalized predictive control scheme. They performed set point tracking of the temperature and the results obtained showed poor tracking at the start of the experiment but excellent tracking towards the end, even with the small possible amount of the data gathered.

Wormsley and Henry (1994) used neural-network models within a model predictive control scheme to control the distillate temperature in a laboratory-scale distillation apparatus separating methanol and water. An exhaustive search method was used for optimization and they obtained good set point and disturbance-rejection results in their study.

Doherty, Williams, and Gomm (1995) used an RBF-based neural network to model an online pH process and used it within a model predictive control scheme to control the pH of the outlet stream. They used a transport lag volume array method to compensate for the dead time in the tubular reactor. They employed their scheme successfully to regulate the pH under various disturbances and used the filter to improve robustness to noise effects. Draeger, Engell, and Ranke (1995) utilized a neural-network-based model predictive control scheme to control pH in a laboratory-scale neutralization reactor. They used the neural network as the nonlinear prediction model in an extended DMC algorithm to control the pH value. The training data set for the neural network was obtained from online measurements of the inputs and outputs of the plant operating under a PI controller. The results obtained for set-point tracking and disturbance rejection cases showed better results than with the conventional PI controller.

Tsen et al. (1996) used a hybrid neural-network that integrates experimental information and knowledge from a mathematical model for control of quality in an experimental batch polymerization reactor. The hybrid model is utilized for identifying the unknown and unmeasured disturbances in the initial charge of the batch reaction, which is formulated in a model predictive control strategy. The strategy was applied on a real experimental system to achieve the desired product conversion in the least possible time.

Recurrent Neural Networks (RNNs)

The use of recurrent neural networks in these model predictive schemes was reported in two cases. MacMurray and Himmeblau (1995) used an external recurrent neural network to predict and control the product compositions in a packed distillation column within the model predictive control strategy. This was done for set point tracking and disturbance rejection studies. They obtained the same results as those obtained using first principle model, but with less computation time when using the neural network model. Tan and VanCauwenberghe (1996) compared three different optimizing methods for the design of an external recurrent neural network predictive controller based on Smith-type prediction. They used this technique successfully to compensate for large time delays in the control of an anaerobic digester process under set point tracking.

Only recently a nonlinear predictive control technique employing neural networks have been implemented, through software called Process Perfector, in an industrial polypropylene plant. The model predictive control techniques utilize a neural network steady state model and a dynamic process model with the dynamic optimization program to perform the control calculations. The objective of the installation was to control the melt flow rate in the polypropylene polymerization reactor. The manage to get good set point tracking results much better than the traditional linear model predictive method (Keeler et al., 1997).

Some researches also utilized the recurrent neural networks in the control systems of real processes. Temeng, Schnelle, and McAvoy (1995) used a recurrent network to model an industrial multi-pass packed bed reactor which is then used in conjunction with an optimizer to build a nonlinear model predictive controllers. The controller was then used to regulate the temperature within the reactor under disturbance rejection cases. The closed loop results they obtained indicate that the neural network-based controller could achieve tighter control than is possible with decentralized single loop controllers.

Table 2.5: Neural network applications in predictive control techniques - simulation implementation

NN Type	System	Objective	Robustness	References
MFFN/Sig	CSTR	Prod. conc.	Dist.	Psichogios and Ungar, 1991
MFFN/Sig	CSTR	Prod. conc.	Set pt./Dist.	Hernandez and Arkun, 1990
MFFN/RBF	Neut.	pH	Set pt.	Hunt and Sbarbaro, 1992
MFFN/Sig	Dis. Column	Prod. conc.	Set pt./Dist.	Willis, Montague, and Morris, 1992
MFFN/Sig	Dis. Column	Prod. conc.	Dist.	Gokhale, Horuwitz, and Riggs, 1995
MFFN/Tanh	Dis. Column	Prod. conc.	Set pt./Dist.	Lee and Park, 1992
MFFN/filter	Dis. Column	Press.	Set pt.	Turner, Montague, and Morris, 1995
MFFN	Digester	Conc./ pH	Set pt./Dist.	Emmanouilides and Petrou, 1997
RNN	Packed Column	Prod. comp.	Set pt./Dist.	MacMurray and Himmelblau, 1995
RNN	Digester	Conc.	Set pt.	Tan and VanCauwenberghe, 1996

Table 2.6: Neural network applications in predictive control techniques - online implementation

NN Type	System	Objective	Robustness	Reference
MFFN/Tanh	Pressure vessel	Press.	Set pt.	VanCan et al., 1995
MFFN/Sig	Tank-in series	Level	Set pt.	Evans et al., 1995
MFFN	Furnace	Temp.	Set pt.	Sheppard, Grant, and Ward, 1992
MFFN/Sig	Dis. Column	Dist. Temp.	Set pt./Dist.	Wormsey and Henrry, 1994
MFFN/RBF	Neut. Reactor	pH	Dist.	Doherty, Williams, and Gomm, 1995
MFFN/Sig	Neut. Reactor	pH	Set pt./Dist.	Draeger, Engell, and Ranke, 1995
MFFN	Poly. Reactor	Prod. Quality	Opt. time	Tsen et al., 1996
RNN/Sig	Packed bed reactor	Temp.	Dist.	Temeng, Schnelle, and McAvoy, 1995

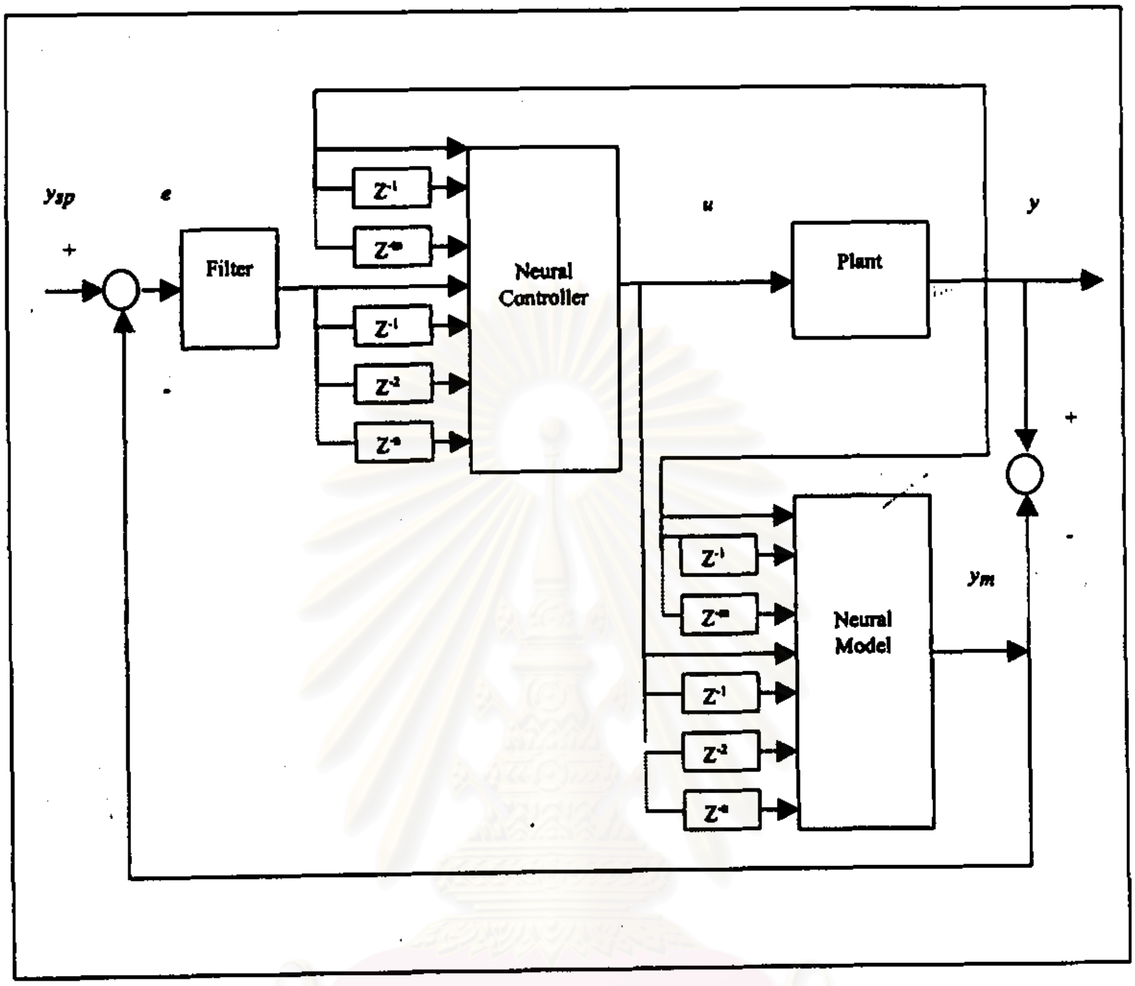

Figure 2.5: Neural networks in internal-model-control strategy.

2.3.2 Inverse-Model-Based Techniques

Two approaches utilizing neural networks in the inverse-model-based strategy are the direct inverse control and the internal-model control (IMC) techniques. In the direct inverse control technique, the inverse model acts as the controller in cascade with the system under control, without any feedback. In this case the neural network, acting as the controller, has to learn to supply as its output the appropriate control parameters for the desired targets at its input. In this control scheme the desired set point acts as the desired output which is fed to the network together with the past plant inputs and outputs to predict the desired current plant input (Pao, Phillips, and Sobajic, 1992). A much more robust and stable strategy is that of the nonlinear internal model control technique, which is basically an extension of the linear IMC method (Economou, Morari, and Palsson, 1986) (see Figure 2.5).

The IMC approach is similar to the direct inverse approach above except for two additions. First is the addition of the forward model placed in parallel with the plant, to cater for plant or model mismatches and second is that the error between the plant output and the neural net forward model is subtracted from the set point before being fed into the inverse model. The other data fed to the inverse model is similar to the direct method. A filter can be introduced prior to the controller in this approach to incorporate robustness in the feedback system, especially where it is difficult to get exact inverse models.

All applications under this category except for two cases reported utilizing multilayer feedforward neural networks in model-based control methods can be seen in Table 2.7 and Table 2.8. They are described in further details later, beginning first with those utilizing the multilayer networks.

<u>Multilayer Feedforward Networks (MFFNs)</u>

Multilayer feedforward networks are widely adopted into many systems, for instance, continuous stirred tank reactor, neutralization, and distillation as provided below.

One of the earliest reported work in process systems was done by Psichogios and Ungar (1991), who utilized an internal model control (IMC) approach to control product concentration in a nonisothermal CSTR with first order irreversible reactions by manipulating the inlet feed temperature. Their control strategy was concerned with disturbance rejection where the disturbance was the change in feed concentration. The inverse-model-based controller was obtained by inverting the neural network model, describing the process dynamics, using Newton 's method numerically. However, they obtained unstable results when the inverse neural network models were directly utilized as the controller in the IMC configuration. Nahas, Henson, and Seborg (1992) also utilized the IMC approach to control the effluent concentration in a CSTR, with first order irreversible exothermic reactions. The inverse model was obtained by numerically solving for the control action, from the formulation of the network forward model. Filtering action and time delay compensation, in the form of a Smith predictor, were also used and offset-free results were obtained in both the set point tracking and disturbance rejection cases. They also implemented the same strategy in controlling the base flow rate. Offset-free results were also achieved here for set point and disturbance rejection cases. Dayal, Taylor, and MacGregor (1994) also implemented the IMC approach for the control of a jacketed CSTR, with first order irreversible reactions, to keep the reactor conversion at its desired setting. A feedback as well as reference model filter was used in this case. In their study they compared the usage of a numerically inverted neural network inverse-model controller for set point tracking as well as disturbance rejection studies. They found that the directly trained neural-network inverse-model as the controller case gave better results overall (except for a slightly bigger oscillation at the step changes) than the numerically inverted inverse-model method, with yet less computational time. They also incorporated a feedforward-feedback strategy to improve on the disturbance-rejection results. However, for the non-monotonic case (i.e. process has well-defined maximum conversion and the steady state gain changes sign) the directly trained neural network inverse-model gave unstable results, which they accounted to the presence of input multiplicity in the reactor behavior. Piovoso et al. (1992) utilized neural networks in the GMC and IMC strategies, respectively, to control the reactor temperature in a first-order, non-adiabatic CSTR system. In the GMC approach, they used a neural network to approximate the functional form of the nonlinear function describing the energy balance, which is required in the controller formulation. In the IMC strategy, they however utilized a PI controller (tuned on a neural network forward model) to estimate the needed control input to produce the required output. They performed set point tracking studies, for the ideal case and with model mismatch, and found that the neural-network-based methods gave comparable results to the pure GMC and global linearizing feedback techniques. Lightbody and Irwin (1995) developed a novel nonlinear model control strategy which utilized the nonlinear neural network model of the plant to act as a medium for the estimation of the parameters of the linear discrete-time model (assumed for the plant). This linear model is then utilized in conjunction with Kalman 's method to design the inverse controller, wherein the parameters of this controller are adapted at each sample instant. They used this approach for set point tracking of concentration in a CSTR system, which outperformed the conventional PID control system. Shah and Meckl (1995) used a neural network in parallel with a proportional controller to control temperature in the CSTR. The neural network they used consists of Gaussian activation function and is trained to learn the inverse dynamics of the CSTR with and without parameter variations. Their simulation results for pseudo-step changes indicate that the neural network can be applied online, even with parameter variation.

Sbarbaro, Neumerkel, and Hunt (1993) utilized the neural network inverse models, acting as a controller, in different ways to control the strip thickness in a steel rolling process, under normal process disturbances. They utilized the inverse model in series with a PI controller, in parallel with an integrator (I) and in the IMC configuration, respectively. Comparisons were also made with the PI and Model Predictive techniques. They found that the inverse model in parallel with the integrator gave the best results but with the IMC and MPC techniques it gave equally good control. In another work with Hunt and Sbarbaro (1992), they utilized multilayer neural networks with radial basis function, in the IMC strategy to perform set point tracking of the pH in a neutralizing reactor. They found in this case that the control system provided very close tracking performance with considerable improvement over a linear controller type.

Ramchandran and Rhinehart (1995) used a neural-network inverse model to estimate the reflux and the holdup rate, which was then incorporated in the Generic Model Control (GMC) strategy to control the top and bottom composition in a distillation column. The GMC technique basically involves incorporating the nonlinear process model directly in the formulation of the control algorithm (Lee and Sullivan, 1988). This was done for set point tracking and disturbance-rejection cases

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Dutta and Rhinehart (1995) used neural-networks to model the steady state inverse of a laboratory-based electrically heated feed preheater system. This was cascaded with a GMC controller in a reference system synthesis approach and used to control the feed temperature of the system. They found that the set point tracking results using this approach were better than the conventional PI and the model-based IMC and MPC approaches.

Hussain, Kershenbaum, and Allwright (1995) utilized a neural-network-based IMC strategy for controlling the temperature of a partially simulated reactor in a pilot plant. They implemented the strategy for set point tracking, disturbance rejection and regulation under plant-model mismatches. The results obtained were found to be comparable with the conventional cascade method with, however, less fluctuations in the control action demanded.

Table 2.7: Neural network applications in inverse-model-based control techniques - simulation implementation

NN Type	System	Objective	Robustness	References
MFFN/Sig	CSTR	Prod. Comp.	Dist.	Psichogios and Ungar, 1991
MFFN/Sig	CSTR	Prod. Comp.	Set pt./Dist.	Dayal, Taylor, and MacGregor, 1994
MFFN/Sig	CSTR	Temp.	Set pt.	Piovoso et al., 1992
MFFN/tanh	CSTR	Prod. Comp.	Set pt./Dist	Nahas, Henson, and Seborg, 1992
MFFN/tanh	CSTR	Conc.	Set pt.	Lightbody and Irwin, 1995
MFFN/RBF	CSTR	Temp.	Set pt.	Shah and Meckl, 1995
MFFN/tanh	Neut.	Prod. Comp.	Set pt./Dist.	Nahas, Henson, and Seborg, 1992
MFFN/RBF	Neut.	pH	Set pt.	Hunt and Sbarbaro, 1992
MFFN/Ellp.	Bioreactor	Conc.	Set pt./Dist.	Aoyama, Doyle, and Venkatasubramanian, 1996
MFFN/Sig	Dis. Column	Prod. Comp.	Set pt./Dist.	Ramchandran, and Rhinehart, 1995
MFFN/tanh	Dis. Column	Prod. Comp.	Set pt.	Basualdo and Ceccatto, 1995
RNN	CSTR	Temp.	Set pt./Dist.	Sbarbaro, Neumerkel, and Hunt, 1993
RNN	CSTR	Conc./Temp.	Set pt.	Nikolaou and Hanagandi, 1993; Scott and Ray, 1993

Table 2.8: Neural network applications in inverse-model-based control techniques - online implementation

NN Type	System	Objective	Robustness	References
MFFN/RBF	Neut.	pH	Dist.	Seborg, 1994
MFFN/Sig	Water bath	Temp.	Set pt./Dist.	Khalid and Omatu, 1992
MFFN/Sig	Semi-batch reactor	Temp.	Set pt.	Dirion et al., 1995
MFFN/tanh	Heater	Temp.	Set pt	Dutta and Rhinehart, 1995
MFFN/sig	partially simulated reactor	Temp.	Set pt./Dist.	Hussain, Kershenbaum, and Allwright, 1995

Recurrent Neural Networks (RNNs)

Nikolaou and Hanagandi (1993) used a recurrent neural network within a state feedback linearizing control strategy to control the temperature of a non-isothermal CSTR system. In this case the recurrent neural network acts as the open-loop observer supplying the network states to the linearizing control formulation. An external linear controller was also applied to the system and the whole strategy, implemented for set-point tracking and disturbance-rejection studies, showed better performance than the linear, optimally tuned controller. Scott and Ray (1993) developed recurrent neural networks (which also have direct connections from inputs to outputs) where the topology and initial weights of the network were determined from an approximate linearized model of the system. These networks were then consequently prune to remove the weights with negligible values and these networks were then applied in various model-based control methods such as the direct control and IMC methods. These methods were applied to the task of controlling both the concentration and temperature of a non-isothermal CSTR under set-point regulation, plant-model mismatches and disturbance-rejection studies. They showed that these neural networks based controllers performed much better than the linear methods in controlling the process over a wide range of conditions.

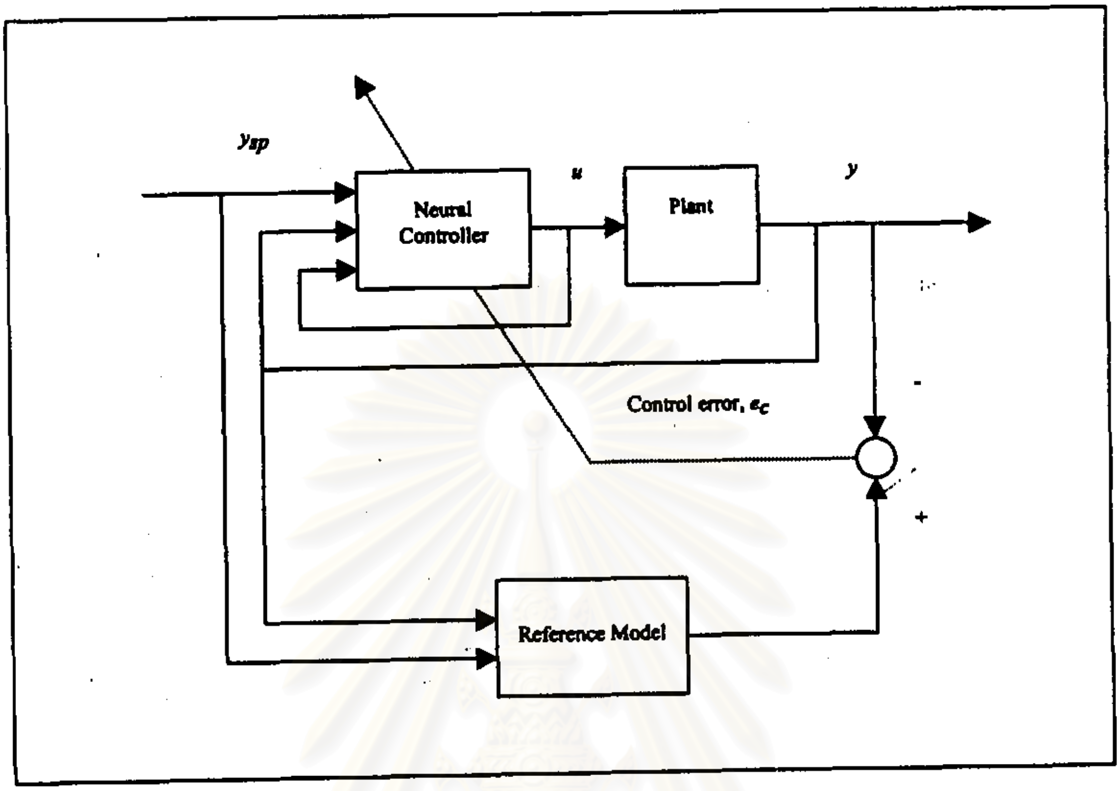

Figure 2.6: Direct adaptive control.

2.3.3 Adaptive Control Techniques

As with other techniques, neural networks can also be adopted into the conventional adaptive control structures in the control of nonlinear dynamic systems. These adaptive methods are normally categorized into two approaches i.e. direct and indirect adaptive schemes. In the direct adaptive control scheme as shown in Figure 2.6, there is no explicit attempt to determine the model of the system; instead the controller parameters are directly adjusted on-line to achieve the necessary tracking and stability of the closed loop system. In this scheme involving neural networks, the weights of the neural network, acting as the controller, are adjusted on-line to control the plant by minimizing some cost function involving the plant output and desired response. A possible adjustment algorithm for the weights of the neural controller can be based on gradient descent such as in the backpropagation technique, which provides the necessary gradient of the cost function with respect to the network parameters (Lightbody et al., 1992). In fact this approach is closely similar to the direct inverse-model control method with the main difference being that the controller is adjusted on-line using a model reference signal in this approach.

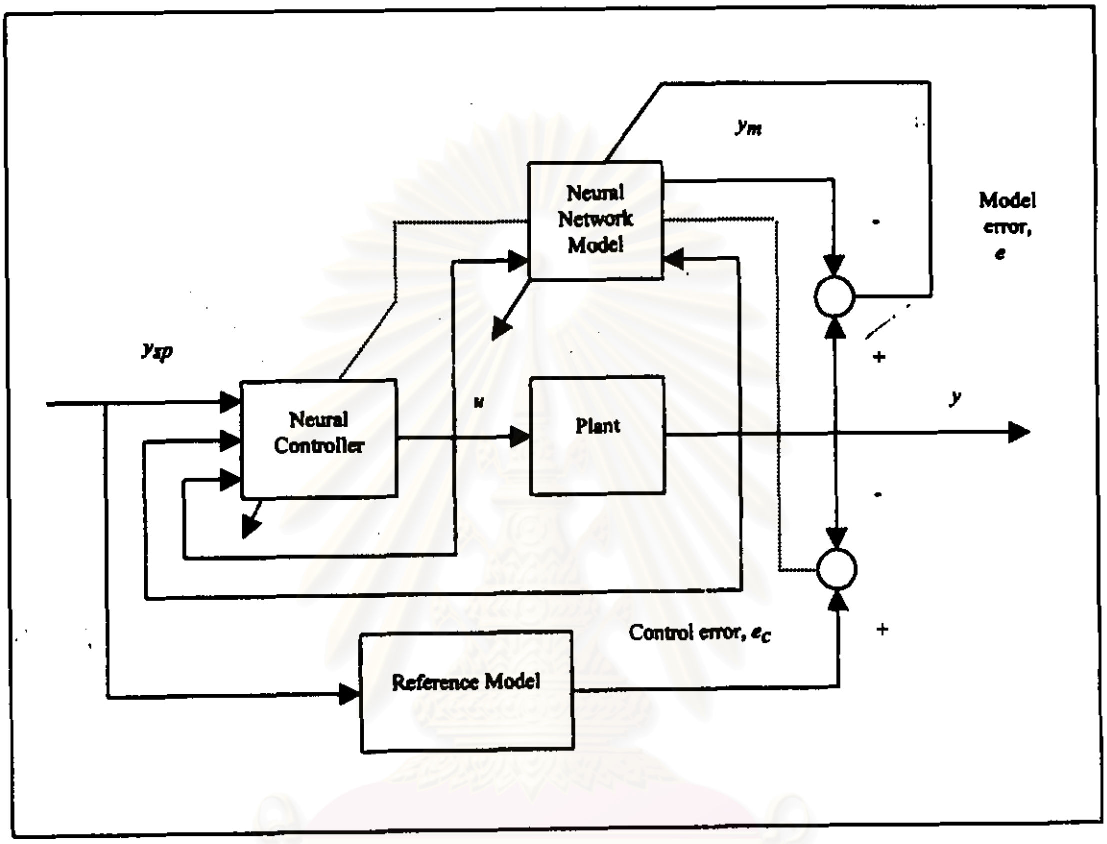

Figure 2.7: Indirect adaptive control.

In the indirect adaptive control scheme as illustrated in Figure 2.7, a neural network is used to identify an unknown/part function of a nonlinear plant online. The objective of the control strategy in this case is to make the plant output follow the reference output. The control action can be then computed from the knowledge of the required output and that of the nonlinear plant, made up of the known function of the model and the neural network model emulating the unknown part/function of this plant. Control action is normally initiated once the plant is identified to the desired level of accuracy so that the output of the plant follows the output of the stable reference model. In this way, both identification and control are performed simultaneously with the time interval for updating the identification and control chosen carefully to achieve stable results. Details of this scheme can be found in seminal paper of Narendra and Parthasarathy (1990). Sanner and Slotine (1992) have also proposed improvement to this basic approach by adding a sliding control term to the neurocontroller, to increase the region of operation.

Most of the applications in this category utilized the multilayer feedforward neural networks are summarized in Table 2.9 and Table 2.10. They are described in further details later.

Multilayer Feedforward Networks (MFFNs)

Ydstie (1990) utilized neural networks in direct adaptive and indirect adaptive control type techniques for a CSTR with second order reactions occurring between sodium thiosulphate and hydrogen peroxide. Their control objective was achieved successfully in making the temperature follow a predetermined reference by controlling the reactant flow rate. In the direct adaptive method, the control action was solved by numerical techniques at each step and implemented as a one-step-ahead predictive method. The network was trained by what they called as the "error-broadcast" algorithm. Lightbody and Irwin (1995) used a neural network in parallel with a fixed gain linear controller in a direct model-reference adaptive control configuration to control the product composition in a CSTR system. Another neural network in parallel to the nonlinear system is used to generate the plant jacobians for updating the neural network controller online. They showed that this method provided greatly improved performances over the conventional PI controller under linear model reference output tracking.

Boslovic and Narendra (1995) applied both the conventional multilayer neural networks and radial basis function networks in an adaptive control scheme, which updates the unknown parameters online, for production of baker's yeast in a fed-batch fermentation process. They considered the set point regulation of the system under no-noise and Guassian noise cases. They found that the conventional multilayer network gave superior performance over the RBF and other nonlinear techniques such as the nonlinear adaptive and inverse dynamics controller. Chovan, Catfolis, and Meert

(1996) used neural networks in a clustered scheme (combination of clusters of neural network controllers and models) within the indirect adaptive control method. They adopted real-time learning with the controller trained by backpropagating the error through the network model. They performed set point tracking for the control of cell mass yield in a bioreactor system with successful results.

Loh, Looi, and Fong (1995) used neural networks in conjunction with a PID in a model reference adaptive strategy to control a process pH. In this case the network consists of a cascade of two single hidden layer nets: the first being a recurrent network to reflect the dynamic nature of the neutralizing reactor and the second net is a static one to reflect the static nature of the titration characteristic. Their results indicated good set point tracking performance even under external load disturbances.

Yang and Linkens (1994) developed an adaptive online neural network-based controller where the neural network controller is adapted online by error signals from the neural network model emulating the plant. The neural network is used to control a bioreactor with time-varying characteristics and nonlinearity. They obtained good results for set point tracking, disturbance rejection and regulation under noisy signals but with extensive computational time.

Watanabe (1994) also utilized an adaptive control scheme where the neural network inverse models acting as the controllers were update on-line in the special inverse and error feedback learning method respectively. These methods were applied successfully in a multiple-input multiple-output (MIMO) continuous polymerization reactor to control the number average molecular weight of the polymer product and the temperature in the reactor under set-point tracking conditions.

Chovan, Catfolis, and Meert (1996) used neural networks in a clustered scheme (combination of clusters of neural network controllers and models) within the indirect adaptive control method. They adopted real-time learning with the controller trained by backpropagating the error through the network model. They performed set point tracking for the control of level in the tank with successful results.

Table 2.9: Neural network applications in adaptive control techniques - simulation implementation

NN Type	System	Objective	Robustness	References
MFFN/Bypass	CSTR	Temp.	Set pt.	Ydstie, 1990
MFFN/Tanh	CSTR	Prod. conc.	Set pt.	Lightbody and Irwin, 1995
MFFN	Neut.	pH	Dist.	Loh, Looi, and Fong, 1995
MFFN	Bioreactor	Cell mass yield	Set pt.	Chovan, Catfolis, and Meert, 1996
MFFN	Bioreactor	Cell conc.	Set pt.	Yang and Linkens, 1994
MFFN	Fermentation	conc.	Set pt.	Boslovic and Mnarendra, 1995
MFFN	Poly. Reactor	MW Prod./ Temp.	Set pt.	Watanabe, 19694
MFFN	Tank	Level.	Set pt.	Chovan, Catfolis, and Meert, 1996

Table 2.10: Neural network applications in adaptive control techniques - online implementation

NN Type	System	Objective	Robustness	References
MFFN/Sig	bench-scale furnace	Temp.	Set pt.	Khalid, Omatu, and Yusuf, 1993
MFFN/RBF	Oven system	Temp.	Set pt.	Dubois, Nicolas, and Billat, 1994
MFFN/Tanh	Process control unit	Flow	Set pt./ Dist.	Noriega and Wang, 1995
RNN	Fermentation	pH	Dist.	Syu and Chang, 1997

For online applications of multilayer feedforward networks, Khalid, Omatu, and Yusuf (1993) used an adaptive neural network controller, where the weights were adapted on-line, to control the temperature within a multiple-input multiple-output (MIMO) bench-scale furnace. The weights were adapted online by backpropagating the error through a forward neural network acting as the emulator. Studies for set point tracking, disturbance rejection and the effects of parameter changes were also done in this case. In both applications they obtained better results than those obtained using the conventional PI controller.

Dubois, Nicolas, and Billat (1994) used an adaptive IMC control strategy, where the model was updated online, to control the temperature in an oven system.

However, they could not get an accurate inverse model from training it with the plant data and resorted to training the inverse model using the data from the neural network model instead. An RBF-based neural network model was used in this scheme to control the oven to follow various desired temperature trajectories satisfactorily.

Noriega and Wang (1995) used a direct adaptive neural network to control the flow rate of a bench-scale flow-process control unit. The control signals in this experiment were generated directly by the well-established gradient descent rule. The system was tested for set point changes with fixed and changing network learning rates and for disturbance-rejection cases with successful results.

Recurrent Neural Networks (RNNs)

Recently, Syu and Chang (1997) utilized a recurrent backpropagation neural network for online adaptive control of a penicillin acylase fermentation process. In enhancing the effective online learning of the network, moving data scheme was supplied to train the network. The pH of the system was well controlled in their experiments with maximum optical density achieved under different types of disturbances.

2.3.4 Neural Network Applications in Other Control Techniques

In addition to three control techniques presented above, there are few online applications implemented neural networks in other control configurations. Multilayer feedforward networks were proposed in their works. Langonet (1993) utilized neural networks to copy the dynamic behavior of conventional controllers, tuned for different operating conditions (corresponding to different valve openings), for the control of the level in a tank by manipulating the output flow. The neural network was able to control the system satisfactorily when switching from one operating condition to another without any need for retuning.

Baratti, Vacca, and Servido (1995) used neural networks to estimate the distillate and bottoms composition of a gasoline stabilizer tower in a refinery plant.

This was utilized for inferential control of the isopentane composition in the column, in conjunction with a PI control system. They found that this method outperformed the normal way of using the temperature for inferential control of the system.

2.4 Other Applications of Neural Networks in Chemical Engineering

Besides the applications in process modeling and control, Neural networks have also been used for other purposes. For examples, they were employed to predict the PID tuning parameters for the auto-tuning of PID controllers (Morris, Montague, and Willis, 1994). Furthermore, they were also incorporated with other types of techniques, such as the cerebellar model articulation controller (CMAC), the B-splines network (Brown and Harris, 1994) and fuzzy systems (Linkens and Nie, 1994).

Inferential estimation is another area where neural networks have proved extremely useful. Measurements from established instruments can be used as secondary variables for estimation of "primary" quality variables. Linear adaptive estimators have been traditionally used to provide fast inferences of variables that are available only less frequently. The use of neural networks might provide improved estimation performances for nonlinear systems. Willis et al. (1991) used neural networks to provide biomass estimation in continuous mycelial fermentation broths. Willis, Montague, and Morris (1992) also obtained biomass estimates from available on-line measurements in a penicillin production process. Baratti, Vacca, and Servido (1995) demonstrated the feasibility of including a neural network model with in a dynamic state variable estimator to construct "software sensors" for two industrial distillation columns that is a butane splitter tower and a gasoline stabilizer. The "software sensors" are capable of reconstructing the full state of the process from incomplete online measurements.

Other applications of neural networks in chemical engineering are summarized in Table 2.11.

Table 2.11: Neural networks in other applications of chemical engineering

Applications	References
Sensor data analysis	Piovoso and Owens, 1991
Fault detection and diagnosis	Venkatasubramanian, 1991; Sorsa et al., 1991; Witoon Suewatanakul, 1993, Fan, Nikolaou, and White, 1993; and Vora, Tambe, and Kulkani, 1997
Sensor failure detection	Naidu et al., 1990
Data rectification and gross error detection	Karjarla, Himmelblau, and Mikkulainen, 1992; Karjala and Himelblau, 1994; and Karjala and Himelblau, 1996
Optimization	Narendra and Parthasarathy, 1991; Chen and Weigand, 1994; Krothapally and Palanki, 1997