CHAPTER II

LITERATURE REVIEW

The purpose of the literature review is to present the basic fundamentals of BD, NN, and MPC. For the first section of this chapter, modeling and optimization of BD column are presented. The second section focuses on issues related to the background of NN. The final section, the basic concept of the MPC is presented.

2.1 Batch Distillation

Many studies on BD have mainly concentrated on developing a model and searching the optimal reflux ratio policies. Some issues considered in the literature are summarized as the following.

2.1.1 Modeling

Simulating the actual operation of conventional columns has been the subject of much research for more than half a century. The main interest was usually to develop a model that could best predict the operation of the column.

Primarily, BD models have been analyzed by short-cut method. Diwekar and Madhaven (1991) modified the short-cut method for a nonideal system. In 1960, Huckaba and Danly presented the first simulation of a BD column. The main assumptions made in the formulation of the mathematical model included binary system, constant weight holdup, linear enthalpy, and adiabatic operation. Meadows (1963) presented the first rigorous multicomponent BD model. The main assumptions being perfect mixing on all trays, negligible vapor holdup, adiabatic operation, theoretical trays, and constant volume plate holdup. Distefano (1968) extended the model and developed a numerical method for solving the equations. Boston et al (1981) further extended the model to efficiently handle the nonlinear nature of the problem. The stiff nature of multicomponent BD equations sometimes requires the use of special numerical methods.

Recently, Jeung Kun Kim and Dong Pyo Ju (2003) developed a rigorous calculation method for a BD operation with a distillate receiver. The validity of the proposed method is confirmed by comparing the simulation results with the experimental data that obtained in the separation of ternary mixture. The authors concluded that the proposed calculation method is useful for separating a nonideal multi–component mixture. Moreover, Bonsfills and Puigjaner (2004) developed model based on mass balances and validated the model with the experiment. The multicomponent was used to studies with satisfactory results.

2.1.2 Optimization

The optimization of a BD column is considered in the literature as *an optimal control policy problem*. The determination of the optimal reflux policies has induced many researchers problem can be classified in the following.

Problem 1: minimum time problem
Problem 2: maximum distillate problem
Problem 3: maximum profit/productivity problem

Converse and Gross (1963) presented the problem 2 for binary system. The optimal policy resulted in the product yield increased by 4 to 5% over the constant overhead composition and constant distillate rate policies.

S. Farhat et al. (1990) developed the optimization of the multiple–fraction separation problem with fixed final time. This is accomplished by simultaneously optimizing the switching times and the reflux policies for each period. The reflux policies are chosen as constant, linear, or exponential in each period. The problem is formulated as a nonlinear programming problem which can be solved either by problem 1 or by problem 2. Three examples have shown that the optimal linear or exponential reflux policies give about 5 to 10% more distillate compared with the optimal constant reflux policy.

The summary of the past work on the dynamic optimization problem is presented in Table 2.1.

Reference	Mixture	Optimization Problem
Converse and Gross (1963)	Binary	Problem 2
Robinson (1969)	Multicomponent	Problem 2
Kerkhof and Vissers (1978)	Binary	Problem 3
Hansen and Jorgensen (1986)	Binary	Problem 1
Farhat et al. (1990)	Multicomponent	Problem 2
Logsdon et al. (1990)	Binary	Problem 1
Diwekar (1992)	Binary and Multicomponent	Problem 1, 2, 3
Logsdon and Biegler (1993)	Binary	Problem 2

 Table 2.1
 Summary of the past work on optimization problem of BD

2.2 Neural Networks

Typically, NNs can be used as a representation framework for modeling nonlinear dynamic systems. Moreover, NNs are also used in many control configurations, for example, MPC, inverse-model based control, and adaptive control. In this work is only concerned the MPC.

2.2.1 NN Modeling

Narenda and Parthasarathy (1990) introduced the models that MFFN and recurrent NN were interconnected in novel configuration for both identification and control. It was found that the NNs could be used effectively for the identification and control of nonlinear dynamical systems.

Pollard et al. (1992) demonstrated that MFFN models could be built for real industrial processes. They conducted experiments on distillation column unit with one input (column reflux flow rate) and one output (tray temperature) and obtained a NN dynamic model. They also demonstrated the utility of cross validation.

Reference	System	NN Application
Song and Park (1993)	CSTR	Modeling and Control
Rohani et al. (1999)	Crystallization	Modeling and Control
Shene et al. (1999)	Batch fermentation	Prediction
Kittisupakorn et al. (2001)	CSTR	Modeling and Control
Chen et al. (2002)	pH neutralization	Modeling and Control
Jha and Madras (2005)	Adsorption	Modeling
Kittisupakorn et al. (2005)	Recovery	Modeling
Georgieva and Azevedo (2006)	Crystallization	Modeling and Control

Table 2.2 Applications of NN

2.2.2 NN MPC

Psichogios and Ungar (1991) utilized a NN 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.

Song and Park (1993) proposed a neural MPC strategy combining a NN for plant identification and a nonlinear programming algorithm for solving nonlinear control problems. The neural model predictive controller showed good performance and robustness.

Wormsiey and Henry (1994) used neural-network models within a MPC 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.

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 nonlinear model predictive controllers. The controller was then used to regulate the temperatures within the reactor under disturbance rejection cases. The closed loop results they obtained indicate that the NN-based controller could achieve tighter control than is possible with decentralized single loop controllers.

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 MPC strategy. The strategy was applied on a real experimental system to achieve the desired product conversion in the least possible time.

Emmanouilides and Petrou (1997) utilized NNs in a model predictive scheme to control the substrate concentration and pH of a complex nonlinear anaerobic digestion system. In his implementation, the NN 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. Recently, Chen et al. (2002) developed a neural MPC for nonlinear processes with unmeasured disturbance.

2.3 Model Based Control

Though the ideas of receding horizon control and MPC can be traced back to the 1960s, interest in this filed started to surge only in the 1980s after publication of the

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first papers on identification command (IDCOM) (Richalet et al., 1978) and dynamic matrix control (DMC) (Cutler and Ramaker, 1980) and the first comprehensive exposition of generalized predictive control (GPC) (Clark et al., 1987).

In 1992, Eaton and Rawlings discussed the MPC, a scheme in which an openloop performance objective is optimized over a finite moving time horizon. MPC is shown to provide performances superior to conversional feedback control for nonminimum phase systems or systems with input constraints when future set points are known. Stabilizing unstable linear plants and controlling nonlinear plants with multiple steady states are also discussed.

Lee (1994) used the successive linearization in nonlinear MPC for technique base on local linear approximation of state/ measurement equations computed at each sample time. The prediction equation is made linear with respect to the undecided control input move by making linear approximations dual to those made for the Extended Kalman Filter (EKF). As a result of these approximations, increase in the computational demand over linear MPC is quite mild. The prediction equation can be computed via non-iterative nonlinear integration. Minimization of the weighted 2norm of the tracking errors with various constraints can be solved via quadratic programming. Connections with previously published successive linearization based approaches of nonlinear quadratic dynamic matrix control are made.)

Schwarm and Nikolaou (1999) showed the robustness of MPC is respected to satisfaction of process output constraints by a closed-loop MPC system that employs an uncertain process model. The method relies on formulation output constraints as chance constraints using the uncertainty description of the process model. The resulting on-line optimization problem is convex.

Rohani et al. (1999) studied linear and nonlinear MPC of a continuous cooling crystallization process, its result shown that the nonlinear MPC provides a satisfactory controller. Moreover, he provided the guidelines for selecting the controller parameter as follows:

Increase in control parameter	Effect on control performance
The output prediction horizon ($N_{PREDICT}$)	Smoothes the outputs and manipulating variables Increase computational time
The manipulated variables horizon $(N_{CONTROL})$	Stabilizes overall control action Increases computational time
The weighting on the output error (W_1)	Improves control performance on the corresponding output Reduces offset
The weighting on the rates of manipulated variables (W_2)	Reduces fluctuations Help decoupling

 Table 2.3
 The effects of control parameters on control performance