CHAPTER I

INTRODUCTION

With increasing need for improving process economics, efficiency and quality, there have been engineering efforts to develop new chemical process designs to improve existing process performance including aforementioned purpose. Combining chemical reaction and membrane separation into a single process unit, one of engineering efforts, is an attractive approach in the chemical industries because of several benefits, for example, enhancing yield, and increasing reaction rate and selectivity.

A pervaporative membrane reactor is a membrane reactor obtained from the integration of pervaporation-based membrane and chemical reactor. The A pervaporation involves the separation of two or more components in liquid mixtures. It is specially used for organic-water and organic-organic separation across a membrane. The concept of the pervaporation is to remove by-product species from reaction mixtures, thus a reversible reaction that produces by-product water, for example, esterification, is a place of reaction enhancement by using the pervaporation. Furthermore, the interesting application of combining the pervaporation with a chemical reactor is to improve yield in a number of equilibrium-limited reactions.

The integration of the pervaporation based on a conventional esterification process that is operated in a batch mode is considered in this work. It is widely accepted that esterification, one of the most important chemical processes in organic chemical industry, is typically a reversible process which its conversion is limited by

thermodynamic equilibriums. Therefore, the coupling of the pervaporation with an esterification reactor is developed to increase the conversion of reactants. That pervaporation can shift the equilibrium by passing water out of a reaction mixture. However, the performance of the pervaporative membrane reactor regarding to permeation rate and reaction rate is still depended on important operating parameters such as the operating temperature and reactant mixtures.

In this work, a neural network inverse model based controller (NIMC) has been designed and formulated to control an optimal temperature of a pervaporative membrane reactor for esterification and its performance has been evaluated in both nominal and plant/model mismatch cases, and compared with GMC coupled with Kalman Filter. In addition, a neural network based estimator has been also embedded in this work to estimate the heat release of chemical reaction.

1.1 Research Objective

The objective is to study the use of neural network, feedforward networks in order to estimate the heat release of chemical reaction, use of neural network as a nonlinear controller, and compare the performance of neural network inverse model based controller (NIMC) with the GMC coupled with Kalman Filter.

1.2 Scope of Research

1. Nonlinear system, Esterification of acetic acid, butanol and batch reactor integrated with pervaporation is utilized in this work. This

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3. A pervaporative membrane reactor has been controlled to achieve a desired objective by using neural network

4. Efficiency of neural network based controller has been compared with GMC coupled with Kalman Filter.

1.4 Activity plan

1. Study the pervaporative membrane reactor and esterification reaction

2. Study the neural networks and simulation program based on MATLAB and MATLAB toolbox.

3. Review relevant information regarding membrane process and membrane reactor including collect the simulation data from mathematical model.

4. Design neural network based estimator to estimate the uncertain parameter. Use simulation data in item 3 to train and test the networks.

5. Design the neural network based controller.

6. Collect and summarize the simulation result.

7. Compare the simulation result of neural networks with GMC coupled with Kalman Filter.

8. Provide discussion and conclusion.

This thesis is divided into six chapters:

Chapter I is an introduction to this research. This chapter consists of research objective, scope of research, contribution of research, and activity plan.

Chapter II presents the literature review in pervaporative membrane reactor and neural networks.

Chapter III describes background information of pervaporation separation process.

Chapter IV describes the neural network fundamentals consisting of biological neural networks, basic neural network, neural network design and application of neural network.

Chapter V presents the configurations of neural network based estimator and controller. The simulation results and discussion are included in this chapter.

Chapter VI presents the conclusion and recommendation for the future work.