CHAPTER 1

INTRODUCTION

1.1 Background of Study

The pH system is very important in world of chemistry especially in chemical industries. In chemistry, pH is a measure of acidity or basicity of a solution. Normally, at pH equal to 7 the solution is called neutral while at pH above 7 is called base and acid solution is vice versa to the base.

There are two different schools of dynamic pH modeling. The first one is the classical physico-chemical modeling approach presented by McAvoy et al. (1972) and the reaction invariant formulation of the physico-chemical approach presented by Gustafsson and Waller (1982). Both approaches are based on same idea of separating the chemical reaction (equilibrium) from the reaction invariant dynamics. The concept of reaction invariant is referred to the conservation of substance on concentrations. The term was originally introduced by Fjeld et al. 1974. In this thesis, the classical physico-chemical modeling approach is used in development mathematical algorithm.

According to Peter Ylén (2001), pH models are divided into two types. The first type is known as static modeling. Static model are valid when the system has reached the equilibrium. The acid-base unit reactions can be considered instantaneous
and therefore static modeling is a very natural approach. Static models include titration curves and distribution diagrams. Experimental static models are often basic tools for product quality control as well as process state indicators. Experimental methods have been used for both qualitative and quantitative analysis.

The second type of pH model is dynamic modeling. Dynamic modeling is more difficult than static modeling. The difference between static modeling and dynamic modeling is it concentrates only on the equilibrium state where the system does not change as a function of time. In the dynamic modeling procedure, the behavior of pH and related phenomena are considered as functions of time. This statement means they will change autonomously even though the changes in the input have already passed. The dynamic pH system can be divided into two categories. First category is when the systems where chemical phenomena are significantly faster than flow and mixing phenomena. The second category is when the system is not in case like category one.

1.2 Problem Statement

pH control is well known as a difficult problem frequently encountered in the chemical process and biotechnology industries. It has been recognized as a challenging problem due to the time-varying and nonlinear characteristics of the pH process. The difficulty arises from the high nonlinearities of the process around the neutralization process. This is true when control has to be achieved in the neutral range (a pH between 6 to 8) when only strong acids and strong bases are present.

Because of the pH process nonlinear characteristic, the linear model cannot predict the process behavior accurately in all operating regions. The steady state gain of pH process shows significant variation with the change of in the operating point. This makes it difficult to design a single linear controller to perform accurately in all the
regions. This is because linear model only acceptable when the process operates at a single set point. The problem is many chemical processes including pH process do not operate at single set points. They are often required to operate at different set points depending on the product needed.

1.3 Objectives of Study

i. Development of mathematical model for pH system based on first principles.
ii. Validation of mathematical model through experimentation.
iii. Simulation studies under steady and unsteady state condition.

1.4 Scope of Study

The scopes of study addressed in this research are:

i. Develop of mathematical model based on first principles
ii. Develop nonlinear model
iii. Nonlinear model validation and analysis
iv. Steady and unsteady state conditions