CHAPTER 1

INTRODUCTION

1.1 Introduction

The aqueous solution of acetic acid (HOAc) is normally produced from many chemical and petrochemical processes, such as in the production of cellulose acetate, terephthalic acid and dimethyl terephthalic. Moreover, reactions involving acetic anhydride either as a reagent (e.g. acetyl actions) or as a solvent (e.g. nitration) can produce a large amount of HOAc containing waste. Examples of such relevant processes include the production of cellulose acetate, an ester group of cellulose used in fiber processing and lacquers and photographic films process, which is typically associated with a 35 wt % aqueous solution of acetic acid as a waste stream. Other important processes involves the synthesis of terephthalic acid and glyoxal which has a relatively by-product of dilute acetic acid stream, typically 65 wt % and 13-20 wt %, respectively. In addition, wood distillation contains lower concentration (1-8 wt %) of acetic acid (Saha et al., 2000).

Recovery of the dilute acetic acid, therefore, becomes important issues due to economic and environmental awareness. Generally, two approaches can be taken to treat the dilute HOAc. One approach is the HOAc dehydration using simple distillation or heterogeneous azeotropic distillation. Distillation is normally uneconomic because of the high costs involving in vaporizing water, which is the most volatile compound and is present in very large proportion but processes a large latent heat of vaporization. A different approach is to convert dilute HOAc into useful chemicals such as acetates by reactive distillation. Reactive distillation column, a combination of reaction and distillation in a single vessel, is receiving increasing attention because of its high potential for process intensification. It is applicable to certain reactions in which the maximum conversion is limited by chemical equilibrium in conventional reactors. It offers various advantages over the conventional approach of reactor followed by separation.

In practice, high purity acetic acid obtained is then used as a raw material in the manufacture of many chemical compounds. The large consumption of the world's production of acetic acid is in the synthesis of vinyl acetate monomer (40- 45 wt %), acetic anhydride (25-30 wt %), acetate esters, i.e. ethyl acetate, *n*-butyl acetate, isobutyl acetate and propyl acetate (15-20 wt %), and terephthalic acid (5-10 wt %). The small extent of the utilization of acetic acid can be found in food industries (5-18 wt %) (Wikipedia the free Encyclopedia).

Recently, a number of research activities are focused on the implementation of a reactive distillation as a promising alternative for the recovery of acetic acid. In comparison with the traditional approach of separation followed by reaction processes as mentioned earlier, performing chemical reaction and separation in a single reactive distillation column offers advantages not only to separate acetic acid from aqueous solution but also to produce a valuable product at the same time, thereby reducing capital and energy costs. By following this approach, the recovery of acetic acid via esterification to product a high valued ester, a common solvent used in chemical industries, has received much attention. The esterification of acetic acid and different alcohols is represented by the equation.

$$\text{Acetic Acid} + \text{Alcohol} \Leftrightarrow \text{Acetate} + \text{Water} \qquad (1\text{-}1)$$

Since esterification is equilibrium limited, the use of the reactive distillation for this reaction system seems to be an attractive method; removing some products from the reaction system can increase reactant conversion. Although many researches has been carried out to study on the esterification of dilute acetic acid using reactive distillations in the past years, the results through experiments and simulations have demonstrated that the performance of reactive distillation in terms of the acetic conversion and the acetate product purity is relative low. To improve the reactive distillation performance, influences of various operating conditions and design parameters should be considered.

In this work, the implementation of a reactive distillation to recover dilute acetic acid via esterification with butanol for the production of butyl acetate, a relatively important solvent is investigated. Simulation studies of the effect of dilute acetic acid concentration on reactive distillation performances in terms of acetic acid recovery and butyl acetate production are implemented using HYSYS commercial software. The model prediction by the HYSYS simulator is validated with experimental data obtained from the literature. The influences of key operating variables on the performance of the reactive distillation are evaluated in order to design the reactive distillation. The control studies of the reactive distillation column base on the obtained optimal column configuration and specifications are also considered.

1.2 Objective of research

The objective of this research is to design and control a reactive distillation for dilute acetic acid recovery to produce butyl acetate from esterification.

1.3 Scopes of research

- Simulate the reactive distillation for the recovery of dilute acetic acid varied from 30 wt % to 100 wt % via esterification with butanol to synthesis butyl acetate using HYSYS software under steady state.
- Study effects of various parameters such as feed location, total stage of reactive distillation, number of reactive section and location of reactive section, reboiler duty, concentration of acetic acid in feed stream, and mole ratio of feed stream on the performance of reactive distillation in order to determine a suitable configuration of the reactive distillation.
- Design reactive distillation configuration of recovery 80 wt% HOAc.
- Two control structures are evaluated via dynamic simulation.