CHAPTER 1

INTRODUCTION

Due to environmental and safety regulations, growing demands on product quality as well as increasingly competitive markets, the continuous improvement of chemical processes and the development of new ones are an important prerequisite for the success of chemical process industries. To a great extent the cost and quality of a product are determined during the early phases of process development, i. e. conceptual design and basic engineering.

In Olefins plants, a large number of equipment and instruments are used to product high quality ethylene and propylene product. One of the units is an acetylene hydrogenation reactor, the primary objective in operating the acetylene hydrogenation reactor is to assure acetylene removal so that that ethylene product will meet its stringent acetylene specification. The secondary objective is to minimize ethylene losses in secondary reactions. Implementing these needs, one then could do a flowsheet modeling of the unit in a process simulator.

Process simulations or mathematical models are widely used by plant engineers and planners to obtain a better understanding of a particular process. These simulations are being used to answer questions such as how can feeding rate be increased, how can yields be improved, how can energy consumptions be decreased, or how should the available independent variables be set up to maximize profit. With an extension of this, process control is essential in process industries to improve safety and product quality as well as to ensure economically optimal and environmentally sound operation. Research activities in the process control group could be divided into three main fields characterized by a close relationship among each other. Consequently, research in the process control group covers the entire field from signal analysis and processes monitoring over control relevant process modeling, model analysis and model-based controller design up to optimization of operation and control-integrated design.

Process flowsheeting is used to sketch out a picture of what the process will look like by using a diagram of the machinery that will be used and how it will all be connected. Process design is usually not done by one person working alone. A team of designers faces several problems when using a computer as a design tool. Current flowsheeting software allows no easily visible way to track the history of the design as it evolves. It is up to the user to keep track of changes they have made, and save different versions as different files with a unique and easy to understand name. Also, a record of design rationale, and explanations for failed designs is usually kept in the designer's private notes, if they are recorded at all. There are a wide range of units that can be used in the chemical process industry, and a fully robust program would support all of them in any combination. Process simulation software is a computer program designed primarily for flowsheet analyses and evaluation. This computing technology allows chemical engineers to investigate existing and proposed process flowsheets for possible optimization or retrofit. A process simulation software or process simulator is a powerful tool in testing out designs with various configurations: flow rates, temperature, pressure, enthalpy, etc. It has built-in unit operations models wherein a user specifies these configurations. It further provides a mechanism for user-added models. It has also a built-in property solver wherein it harnesses several equations of states to arrive at a reliable physical and chemical property calculations. A process simulation software is capable of performing important and complicated tasks: do steady-state and dynamic simulation of several unit operations and unit processes, perform costing and economic analysis, conduct design optimization based on specified criteria, and enable data-fitting for synchronizing proposed design with realistic data. Process simulation software has some special features added to it by its manufacturer. Some manufacturers may even offer customized design. And each is marked with a unique graphic user interface.

The difficult task of controlling the acetylene impurity product is compounded to the accompanied hydrogenation of the valuable ethylene product to ethane. The quantity of ethylene converted to ethane can be significant. It is estimated that the improper operation of an acetylene reactor in a olefins plant can result in ethylene losses of as much as 2 to 3 percent. For a billion pound per year ethylene plant, this means an annual loss of three million dollars. Thus, the selection of the operating conditions are required to minimize the undesirable hydrogenation of ethylene to ethane, while maintaining the impurity specification on the outlet acetylene.

1.1 Research Objectives

The objective of this thesis are:

1. To develop a steady state process model of a front-end acetylene hydrogenation reactor using commercial process simulator
2. To optimize the process model obtained from (1) to maximize ethylene gained
3. To carry out sensitivity analysis of process parameters affecting the optimum condition

1.2 Scope of Research

The research was divided into three main parts: process modeling, process optimization and sensitivity analysis. The details of particular process are described as follows:

1.2.1 Process Modeling

Aspen Plus Simulation Package was used to create basic and detailed models of the process unit. The basic model was for initial modelling of the process unit. It was also used to verify the input as well as to control parameters to match the model within the study range. In order to complete the whole range process, detailed model was developed to simulate and capture the process within a lesser error range, producing higher and accurate prediction of the unit. Purposely, the effect of feeding temperature and mole fraction components in the feeding stream were investigated using the process model previously developed. Many kinetic reaction models tested against plant data were investigated from several studies reported in literatures. A least square based data reconciliation algorithm in Aspen Plus Simulation Package, using the SQP optimization algorithm, was used to adjust the kinetic reaction model. After evaluations of those, the best model was selected for this study.

1.2.2 Process Optimization

In this study, the process model obtained from the Aspen Plus Simulation Package was used for process optimization in order to obtain the optimal set of plant operation conditions. An objective function was created based on net ethylene gain from operation. Possible variables were hypothesized and then selected for optimization. The process model was then used to obtain the optimal set of plant operation conditions. The SQP optimization algorithm was employed to adjust the manipulated variables to achieve maximum net profit.

1.2.3 Sensitivity Analysis

After a process optimization, a sensitivity analysis study was carried out to check the results, and examine the sensitivity of changes in the coefficient in the problems and the assumptions. The reason to do a sensitivity analysis was that the optimum condition might not be the best in the region of operation due to that a wider range of variables might not be included or mistakenly reported. Also, the result could show a significant importance of the variables to the optimum condition in such a way the process characteristic was better understood. Parameter values usually contain errors or uncertainties in nature. Therefore, information concerning the sensitivity of the optimum changes or variations in a variable is very important in optimal process design.

1.3 Importance of This Research

In general, there are many typical problems in chemical engineering process design or plant operation. Nevertheless, a great number of possible solutions could be found and employed to overcome those constraints. Optimization is concerned with selecting the best variable by efficient quantitative methods. Computer and associated software make the computation involved in the selection feasible and cost-effective. Modeling software such as Aspen Plus Simulation Package could be employed and later on utilized as a tool to obtain an optimization study of the model. In plant operations, benefits arise from improved plant performance such as improved yields of desired products (yield reduction of contaminants), reduction of energy consumption, obtaining higher processing rate, and yielding longer times between shutdowns. Optimization could also lead to maintenance costs reduction, less equipment wear and efficient staff management. Therefor, it is extremely helpful to systematically identify the objective function, operation constraints, and degrees of freedom in a certain process, leading to such benefits as improved quality of design, faster and more reliable trouble-shooting and efficient decision-making. These factors related to optimization operation are very crucial for one who aims the best result and thus lead to initiation of this research project.

1.4 Time Frame

1. Literature review and studies related to the research including Aspen Plus Simulation Package and its ability to serve as the supporting ground to propose this thesis
2. Development of the model as an Acetylene Hydrogenation Unit from design data
3. Modification of the obtained Acetylene Hydrogenation model using Aspen Plus Simulation Package compared with run result with plant data
4. Testing of the Acetylene Hydrogenation Unit model with other sets of data by using Data Reconciliation to adjust the process variables
5. Operation of optimization to obtain the expected optimum condition
6. Carrying out sensitivity analysis study of process parameter affecting the optimum condition
7. Summarizing research data, putting up the remark and making conclusion of the research

Table 1.1 Time Frame

	1998				1999				2000				2001	
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2
1														
2														
3														
4														
5														
6														
7														