CHAPTER 7

CONCLUSION AND RECOMMENDATION

7.1 Introduction

In this chapter, a conclusion and recommendation of the study carried out will be concluded covering the steps, results and conclusion achieved. The early stages of developing the model from design base case. Then, attempts of data fit and reconciliation of the model to actual operation data and last the optimization and sensitivity analysis of the model.

7.2 Base Case Development

In this stage a study of the acetylene hydrogenation process including types, reactions, and base design concepts has been made to develop an understanding of the processes characteristic ad objective in order to develop a model in a flow sheet simulation package, Aspen Plus, as accurate as possible. The acetylene hydrogenation reactor itself is a plug flow reactor, a combination of three reactors connected in series in order to achieve the objective of removing the acetylene which is considered contamination in the ethylene polymer grade production to a level of 1 ppmv. The model used to represent the process in Aspen Plus was a RPLUG and CSTR reactor modules. The kinetic model was study based on the Langmuir-Henshelwood kinetic concept resulting a simplified power-law kinetic model. The power-law kinetic model was adequate enough to represent the reaction occurring within the reactor. Within the power-law kinetic model, the Arrhenius pre-exponential factor was focus and adjusted to fit the model effluent result with the base case effluent information. With this, in was noted that the catalyst deactivation term was lumped with the Arrhenius pre-exponent factor for each reaction rate. The thermodynamic used was the Peng-Robinson which was suitable for a non-polar or mildly polar mixtures. The result of the base case model

was capable of predicting the effluent composition lesser than 0.1 percent average. The prediction of temperature however, was large due to that the design effluent temperature was over 126 °C.

Reviews stated that the rate of ethylene hydrogenation does not depend on the concentration of acetylene as previously reported by Margitfalvy et al. (1981). The explanation may be found in the presence of CO. As pointed out by Bos and Westerterp. (1993a), CO may suppress the influence of acetylene in ethylene hydrogenation. Another surprising feature is the positive values for the adsorption energy on the CO and H_2 constants which indicated that the will increase with temperature. It is reasonable to expect that the adsorption term decrease with temperature due to the exothermic character of the adsorption processes. This anomalous result may be due to data error, inadequate selection of operating conditions, or data analysis. Problems of this kind are often encountered on rate modeling as discussed by Doraiswamy and Sharma (1984). In spite of this difficulty the hydrogenation rates predicted by the model exhibits a normal Arrhenius behavior because the effect of temperature on the adsorption parameters is overcompensated by the large activation energy on the rate constants k_A and k_E. The rate of acetylene hydrogenation is initially larger than that of ethylene, as the reaction proceeds, the decrease in acetylene concentration is compensated by the increase in temperature, so the rate is nearly constant at the 325-340 K. The presence of CO prevents the hydrogenation of ethylene up to a very high level of acetylene conversion. Consequently, a two-site mechanism that may be relevant under different experimental conditions was not used here to obtain additional kinetic equation.

7.3 Data Fit and Reconciliation

After obtaining an agreeable base case model, a data fit and data reconciliation algorithm is used to fit the model by adjusting the pre-exponent factor of all four reaction in all three reactors to match the actual plant operation data. Data from the process is obtained from both laboratory and online gas chromatography. In the fitting process, and study of weights that is applied to the confidence data such as the acetylene concentration was applied. A result shows that the weight should be applied to leverage the mole concentration of the components in order to fit the model correctly and within

an acceptable range. A recommendation of weight applied to acetylene concentration would be 1000. Also, a weight could also be employed with MA and PD concentration. The effluent temperature of all the reactors, especially the lead reactor should be taken notice when implementing the model to simulate actual plant characteristic. Results of the study shows that an over prediction of 4-5 ^{o}C was obtained. This could happen from an over prediction of acetylene hydrogenation, due to usage of the same pre-exponential factor during the simulation over the period of six months. Also, another reason would be that the kinetic parameters used in this model were not accurate enough to predict a closer effluent temperature.

A study was also made to develop a CSTR combined in series to represent a Plug flow reactor. The number of CSTRs was evaluated to obtain a total of the equal size CSTRs connected in series having a total volume equal to the plug flow reactor. A total of 10 CSTR was used to and was found that the performance was nearly the same as a single plug flow reactor. Both the plug flow and the CSTR model is then used to tested with other sets of data to verify the consistency and ability of the model to be used, the result shows that the model could only be used in a certain limit range of time. A recommendation of a monthly renew of the pre-exponential values should be employed.

A pre-exponent factor of the reaction was then carried out to study the changes of it over the operation period. The catalyst activity is resembled by the Arrhenius pre-exponent factor. The result shows that the lead reactor is the most active and the guard reactor is the less active among all of the reactors. A slight decrease of the pre-exponent factor over the operation period was discovered supporting the theory of catalyst deactivation that was lumped by the pre-exponential factor. The catalyst deactivation was studied to determine the effect of catalyst deactivation. The lumped parameter obtained was a function of the catalyst deactivation and the pre-exponential function.

7.4 Optimization and Sensitivity Analysis

An optimization of the model after data fit and reconciliation was made to acquire the optimum operation condition for the acetylene hydrogenation reactors.

Primary, the simulation result of the actual model indicated an ethylene loss of 504.56 kg/hr. The study shows that the major unit producing the ethane was from the

intermediate and guard reactor. The process and list of all the variables in the process was observed. The determination of the criteria for optimization was initiated to maximize the ethylene gain, minimize the ethane production. Results shows that an increment of lead inlet temperature from 68.6 °C to 69.2 °C promotes a larger acetylene conversion in the lead reactor. After employing the optimum operation conditions, an ethylene gain of 43.6 kg/hr could be achieved.

The study shows that the optimum scheme would be to increase the lead inlet temperature and reduce the intermediate and guard inlet temperature. Supported by operation information that the lead reactor is packed with fresh catalyst effecting a good conversion and selectivity of acetylene to ethylene and ethylene to ethane. An increase in the lead inlet temperature could however, shorten the catalyst life that should future be investigated and studied.

The sensitivity study shows the behavior and characteristic of acetylene hydrogenation reactors to disturbances such as changes in acetylene inlet concentration, feed flow rate and lead inlet temperature and the effect of it to the optimum condition. The result shows that 10% increment of the acetylene in the feed stream leads to a higher inlet temperature for the lead reactor in order to achieve the specification of the effluent of the guard reactor. Trials of sharing the loads were made and results were shown that the lead reactor plays the most objective of this whole unit of removing the acetylene component from the feed stream.

A 10% increment was studied in order to simulate a situation when all of the inlet component composition increased. Results indicated that a higher lead inlet temperature ensures the product specification with little adjustments to the intermediate and guard inlet temperature. Results obtained from another study by combining both a 10% increment of acetylene composition and 10% increment of feed flow rate shows a similar result of increasing the lead inlet temperature and a slight increase in the intermediate reactor. The optimum philosophy obtained was that the lead reactor should convert nearly 90% to 95% of acetylene to ethylene in order to remain on specification. The intermediate and guard reactor's objective was to ensure that the acetylene in the outlet stream was below 1 ppmv.

A study of the changes in inlet temperature was made to verify the characteristic of the model and bounds of the operational range.

7.5 Future Studies

Future studies of the model would be to study the Arrhenius pre-exponential factor, the research lumped the reaction rate constant with the catalyst deactivation in order to obtain a catalyst deactivate profile that could be useful for operation practice to switch the reactors.

An addition of other reactions occurred in the reactor, of which is a minority and mostly undesirable, could lead to a better effluent temperature prediction. Literature reviews provides little information regarding the minor reaction, of which laboratory and vendor information should be employed to obtain such information.