CHAPTER 9

DISCUSSION AND CONCLUSION

9.1 Introduction

This chapter, the developed model of the acetylene hydrogenation process, the developed dynamic data reconciliation program for the acetylene hydrogenation process, and the designed Dynamic Matrix controller have been reported to be highly successful. The current study demonstrates the effectiveness and useful of all developed program.

9.2 The simulation model of the acetylene hydrogenation process

In this thesis, the study focuses on the modeling of the acetylene hydrogenation process by using the SPEEDUP program. The acetylene hydrogenation process is comprised of three fixed-bed reactors, pre-heated system, and two inter-cooler systems The developed model is the semiempirical model, the catalytic fixed-bed reactors are approximated by the number of CSTRs that is connected in series, and the rate constant parameters of the models are estimated by using the reconciled data of the actual data from an industrial plant.

For adequate model selection and realistic modeling, the predicted results of simulation especially in the profile of temperature in each bed, more over, the simulated results of output variable are compared with the actual data.

The suitable model of acetylene hydrogenation reactor is approximated by the twenty CSTRs that is connected in series. The four main reaction have the rate laws that are based the following assumption

    1. The rate limiting step is a surface rate of reaction.

    The rate of reaction are :

$$-r_{Ac} = k_{Ac}\theta_{Ac}\theta_{H2}$$

$$-r_{Eth} = k_{Eth}\theta_{Eth}\theta_{H2}$$

$$-r_{MA} = k_{MA}\theta_{MA}\theta_{H2}$$

$$-r_{PD} = k_{PD}\theta_{PD}\theta_{H2}$$

2. The hydrogen breaks into free atom.

3. The product dose not be adsorbed on the catalytic surface.

4. The catalyst activity equation is

$$activity = 1/(1+K_{activity}\Sigma Ac)$$

And the reaction rate equations are

$$-r_{Ac} = k_{Ac}C_{Ac}C_{H2}^{0.5}/(1+ K_{Ac}C_{Ac}+ K_{Eth}C_{Eth}+ (K_{H2}C_{H2})^{0.5}+ K_{CO}C_{CO})^2$$

$$-r_{Eth} = k_{Eth}C_{Eth} C_{H2}^{0.5}/(1+ K_{Ac}C_{Ac}+ K_{Eth}C_{Eth}+ (K_{H2}C_{H2})^{0.5}+ K_{CO}C_{CO})^2$$

$$-r_{MA} = k_{MA}C_{MA} C_{H2}^{0.5}/(1+ K_{Ac}C_{Ac}+ K_{Eth}C_{Eth}+ (K_{H2}C_{H2})^{0.5}+ K_{CO}C_{CO})^2$$

$$-r_{PD} = k_{PD}C_{PD} C_{H2}^{0.5}/(1+ K_{Ac}C_{Ac}+ K_{Eth}C_{Eth}+ (K_{H2}C_{H2})^{0.5}+ K_{CO}C_{CO})^2$$

$$-r_{CO} = k_{CO}C_{CO}$$

Where the estimated rate constant values are

Table 9.1 The proper estimated reaction rate constants

Rate constant	Bed I	Bed II	Bed III
k_{Ac}	4.651236e11	6.351236e11	2.983236e12
k_{eth}	1.886755e13	2.266055e13	2.624055e13
k_{MA}	5.120408e11	7.200408e11	3.815408e12
k_{PD}	6.448e24	7.75e24	9.851e24
k_{CO}	7.248314e-7	6.65514e-8	4.190915e-8
$k_{activity}$	2.586304e-5	2.312045e-5	9.987904e-6

The suitable model provides the certain results of the predicted output variable value as illustrate as follow

♦ The prediction error of the outlet temperature of bed I is 0.13%

♦ The prediction error of the outlet temperature of bed II is 0.25%

♦ The prediction error of the outlet temperature of bed III is 0.23%

♦ The prediction error of the outlet acetylene concentration of bed I is 6.9%

♦ The prediction error of the outlet acetylene concentration of bed II is 7.79%

♦ The prediction error of the outlet acetylene concentration of bed III is 4.41%

♦ The prediction error of the outlet ethylene concentration of bed III is 2.87%

♦ The prediction error of the outlet methyl acetylene concentration of bed III is 14.81%

♦ The prediction error of the outlet propadiene concentration of bed III is 13.43%

Moreover, the model can more effectively repeat the process at current operation by adding the real time parameter estimation.

9.3 The dynamic data reconciliation program of the acetylene hydrogenation process

The chosen method of dynamic data reconciliation is based on weight least square principle. This method is described in the efficient data reconciliation and estimation for dynamic process using nonlinear programming techniques paper by Liebman and friends(Liebman et. al., 1992) and is presented in the thesis in Chapter 3. The dynamic data reconciliation objective function is to minimize the sum of square error between the measurement data and the reconciled data, and the reconciled data must satisfy the material and energy balance equations of the process by adding the material and energy balance constraints. The method that used to solve the objective function under the constraints is the Lagrange Multiple method.

For adequate the history horizon selection, the value of the history horizon is varied, and, the predicted results and computation time of each simulation with different H values are compared.

The suitable history horizon is ten-step of sampling time. The developed dynamic data reconciliation program with H = 10 can reduce the standard deviation of the simulated data decreasingly about 90 %, can reduce the standard deviation of the actual data decreasingly about 40-70 %, but cannot erase or reduce the bias. To erase the bias, the bias estimator must be added and erase the bias from the measurement data before passing the data to the dynamic data reconciliation step.

Moreover, the testing of the capability of the data reconciliation illustrates the improving model accuracy.

9.4 The Dynamic Matrix Control design of the acetylene hydrogenation process

The control objective of an acetylene hydrogenation process is to remove acetylene from ethylene product, to maintain the level of acetylene in ethylene product at 0.1 ppm. The outlet acetylene concentration can be controlled by control the inlet temperature but the temperature is more effectively to the reaction. Thus, the change of temperature value should be slowly and little. The pre-heated system is added in the process for this reason. The pre-heated system comprises of one control valve and one heat exchanger. The inlet temperature that is controlled by the by-pass flow between the valve and the heat exchanger is changed slowly. On the other hand, can say that, the acetylene concentration is controlled by the control the by-pass flow of the pre-heated system.

The Dynamic Matrix controller can be easily designed from the convolution model of the process between the outlet acetylene fraction and the valve position. The convolution model can be found out through the open loop relationship between both of variables. The best Dynamic Matrix controller design is achieved by varying the turning parameters of the controller (V, U, Δt), simulating each program, and then looking for the one that given the best performance in the sense of control.

The suitable Dynamic Matrix Control design is the controller with the control horizon U = 3, the prediction horizon V = 2, sampling time = 7 seconds, and the control weight = 1000. For the even of the total mass flow change, the selected DMC controller gives

- ♦ The shortest setting time = 21.6 seconds that is about 18.4% over the value of PID controller
- ♦ The smallest overshoot = 0.0013 ppm that is about 39.4% over the value of PID controller

♦ The amount of acetylene that passed out with the product is reduce by 96% over by using PID controller

The selected DMC controller gives the good control action in all of the difference evens. The selected DMC controller takes the shorter time to achieve the set point of the controller than the PID controller. The selected DMC controller can reduce the amount of ethylene loss if compares with the PID controller.