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APPENDIX A

Process Stream Data and Equipment Data

Table A1 Process stream data

	Fresh ethylene	Fresh oxygen	fresh acetic acid
Vapour / Phase Fraction	1.0000	1.0000	0.0000
Temperature [C]	30.00	30.00	30.00
Pressure [psia]	150.0	150.0	150.0
Molar Flow [gmole/min]	780.00	460.00	680.00
Oxygen	0.0000	1.0000	0.0000
CO2	0.0000	0.0000	0.0000
Ethylene	0.9990	0.0000	0.0000
Ethane	0.0010	0.0000	0.0000
VinylAcetate	0.0000	0.0000	0.0000
H2O	0.0000	0.0000	0.0000
AceticAcid	0.0000	0.0000	1.0000

	Reactor inlet	Reactor outlet	FEHE hot outlet
Vapour / Phase Fraction	1.0000	1.0000	1.0000
Temperature [C]	148.56	159.50	134.00
Pressure [psia]	123.0	90.0	89.0
Molar Flow [gmole/min]	19507.10	19161.95	19161.95
Oxygen	0.0789	0.0572	0.0572
CO2	0.0051	0.0086	0.0086
Ethylene	0.5847	0.5575	0.5575
Ethane	0.2101	0.2139	0.2139
VinylAcetate	0.0042	0.0403	0.0403
H2O	0.0088	0.0484	0.0484
AceticAcid	0.1082	0.0742	0.0742

Process stream data**(continued)**

	Absorber vapor in	Absorber vapor out	Absorber liquid out
Vapour / Phase Fraction	1.0000	1.0000	0.0000
Temperature [C]	74.23	53.04	66.67
Pressure [psia]	128.9	128.0	128.8
Molar Flow [gmole/min]	16487.19	16261.92	981.19
Oxygen	0.0665	0.0674	0.0001
CO2	0.0100	0.0101	0.0002
Ethylene	0.6474	0.6559	0.0066
Ethane	0.2484	0.2515	0.0027
VinylAcetate	0.0163	0.0050	0.1866
H2O	0.0066	0.0013	0.1474
AceticAcid	0.0048	0.0087	0.6562

	Absorber side stream out	Ethane Purge	Carbon dioxide Purge
Vapour / Phase Fraction	0.0000	1.0000	1.0000
Temperature [C]	48.16	53.15	40.40
Pressure [psia]	128.4	124.5	125.5
Molar Flow [gmole/min]	14999.98	3.00	65.06
Oxygen	0.0001	0.0681	0.0000
CO2	0.0004	0.0000	1.0000
Ethylene	0.0118	0.6626	0.0000
Ethane	0.0049	0.2541	0.0000
VinylAcetate	0.3107	0.0051	0.0000
H2O	0.0706	0.0013	0.0000
AceticAcid	0.6015	0.0088	0.0000

Process stream data**(continued)**

	Carbon dioxide removal in	Column feed	Column bottom
Vapour / Phase Fraction	1	0.0062	0.0000
Temperature [C]	53.04	50.18	124.95
Pressure [psia]	127.0	18.5	19.7
Molar Flow [gmole/min]	6411.00	3655.96	2188.94
Oxygen	0.0674	0.0001	0.0000
CO2	0.0101	0.0002	0.0000
Ethylene	0.6559	0.0042	0.0000
Ethane	0.2515	0.0019	0.0000
VinylAcetate	0.0050	0.1875	0.0000
H2O	0.0013	0.2631	0.0930
AceticAcid	0.0087	0.5431	0.9070

	Wash acid feed in absorber	Organic product	Aqueous product
Vapour / Phase Fraction	0	0.0000	0.0000
Temperature [C]	25.00	38.01	38.01
Pressure [psia]	128.0	18.0	18.0
Molar Flow [gmole/min]	756.00	826.00	729.56
Oxygen	0.0000	0.0000	0.0000
CO2	0.0000	0.0003	0.0000
Ethylene	0.0000	0.0052	0.0001
Ethane	0.0000	0.0026	0.0000
VinylAcetate	0.0000	0.9399	0.0042
H2O	0.0710	0.0518	0.9957
AceticAcid	0.9290	0.0003	0.0000

Table A2 Process equipment data

Reactor	
Length	10 m
Diameter	0.037 m
Number of Tubes	622
Wall Thickness	0.005 m
Reactor heat duty	2.147×10^6 kcal/h

Vaporizer	
Diameter	2.435 m
Height	3.652 m
working level volume	4.00 m ³
vaporizer temperature[C]	119.0
vaporizer heat duty	1.167×10^6 kcal/h

Feed effluent heat exchanger	
FEHE UA	6621 kcal/hC
FEHE hot outlet temperature	119.0 C
FEHE duty	4.195×10^5 kcal/h

Separator and Compressor	
Diameter	2.335 m
Height	3.503 m
working level volume	8.00 m ³
separator cooler duty	2.590×10^6 kcal/h
Compressor size	394 Kw
Gas loop volume	170 m ³

Process equipment data**(continued)**

Absorber	
Base volume	8.00 m ³
Bottom section	2 theoretical stages
Top section	6 theoretical stages
recirculation cooler duty	3.326*10 ⁵ kcal/h
Wash acid cooler duty	8.090*10 ⁴ kcal/h

Column and Decanter	
Theoretical stages	20.000
Feed stage	15 from bottom
Base working volume	8.70 m ³
Decanter base working volume	13.00 m ³
Reboiler duty	4.065*10 ⁶ kcal/h
condenser duty	3.867*10 ⁶ kcal/h

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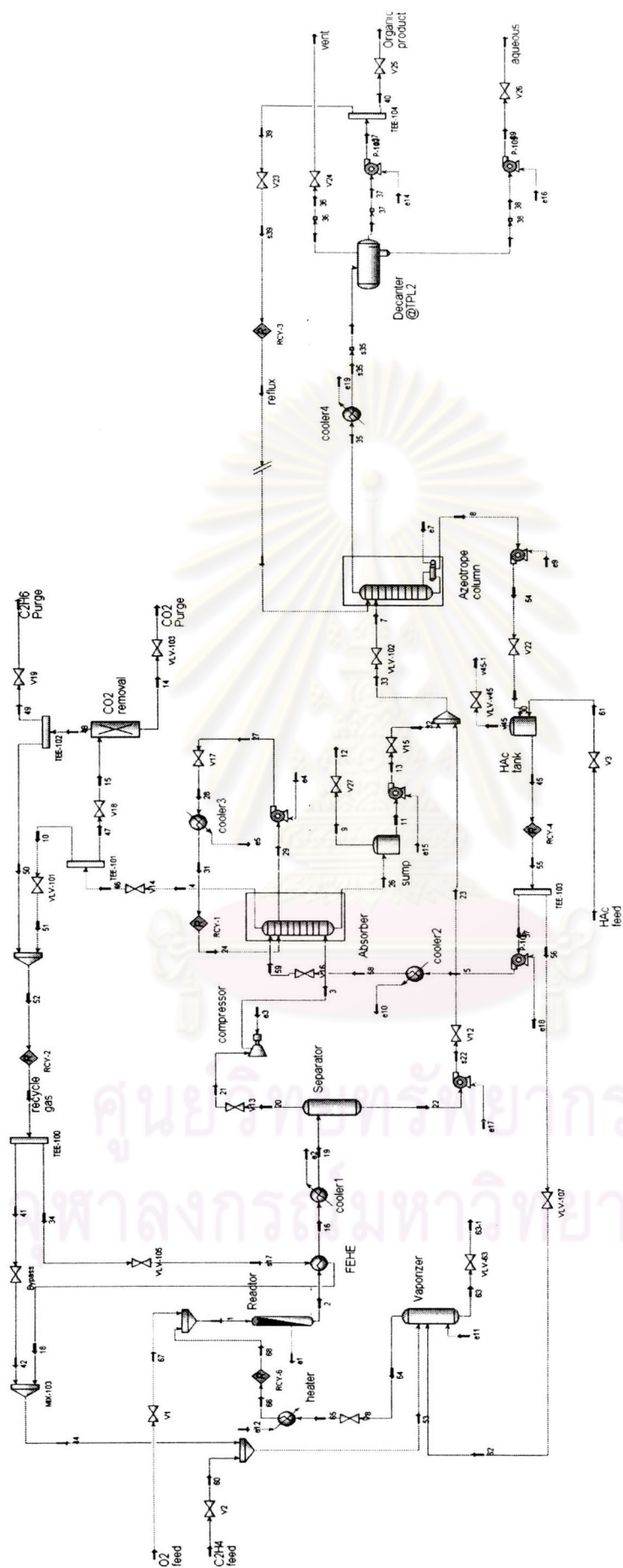


Figure A1 Vinyl Acetate Process flowsheet

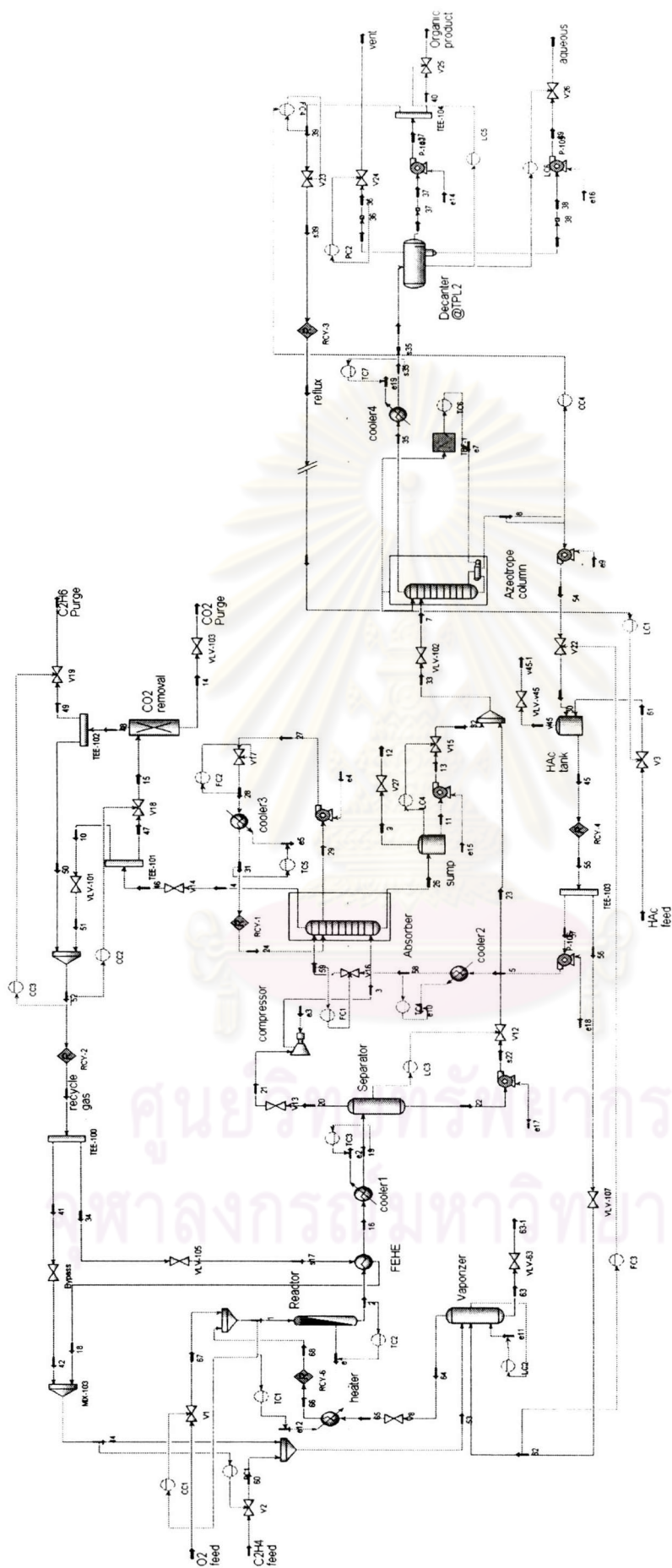


Figure A2 Reference control structure (CS1) of Vinyl Acetate Process

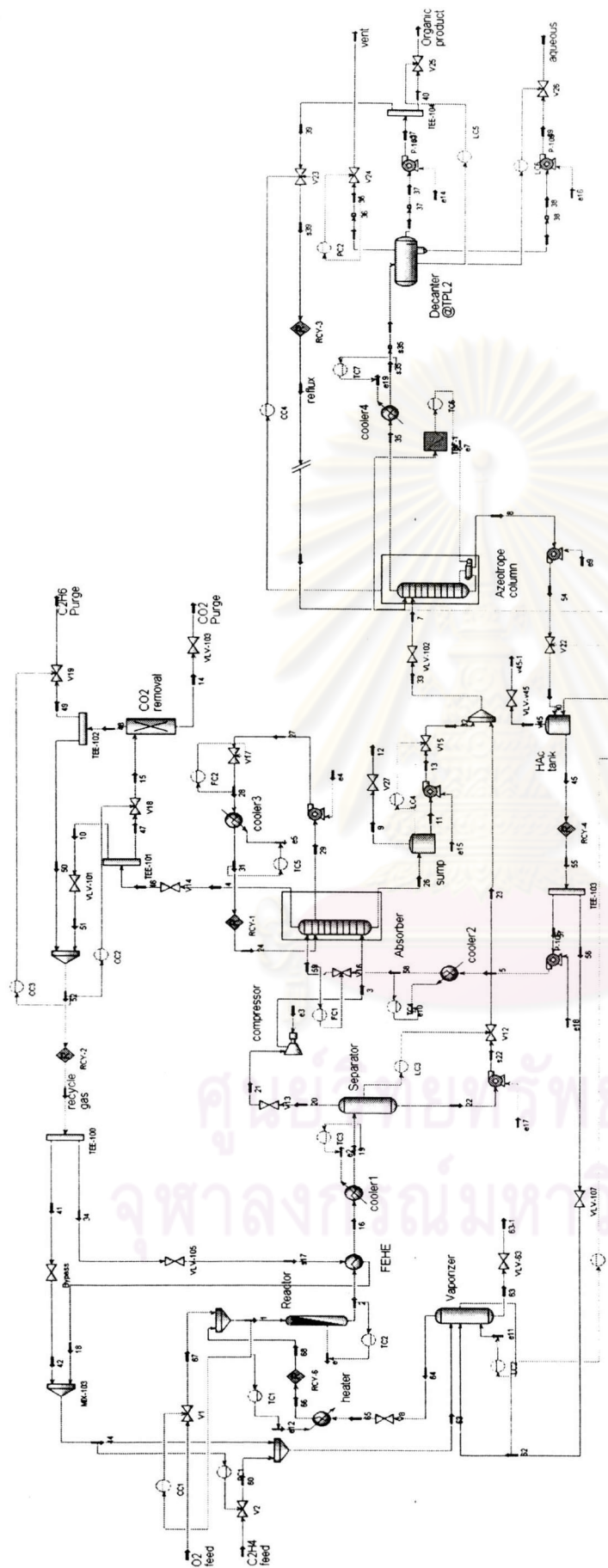


Figure A3 Designed control structure I (CS2) of Vinyl Acetate Process

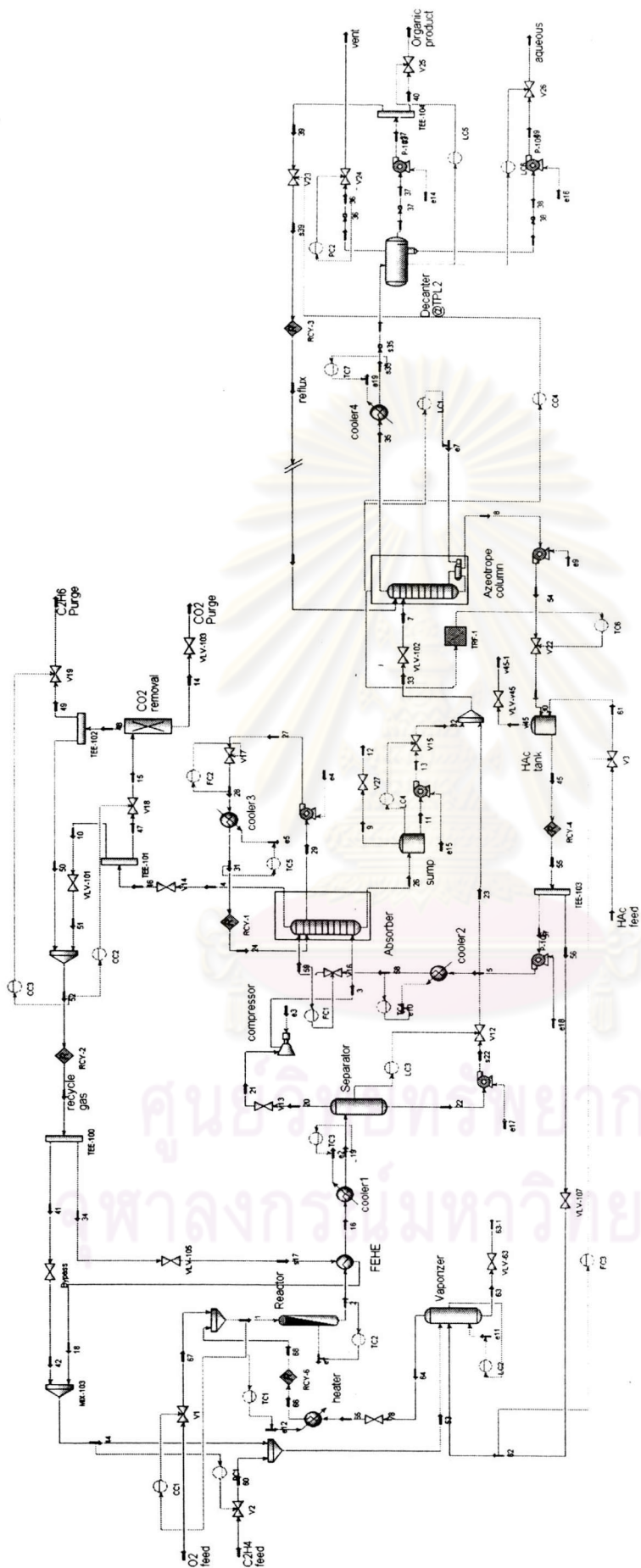


Figure A4 Designed control structure II (CS3) of Vinyl Acetate Process

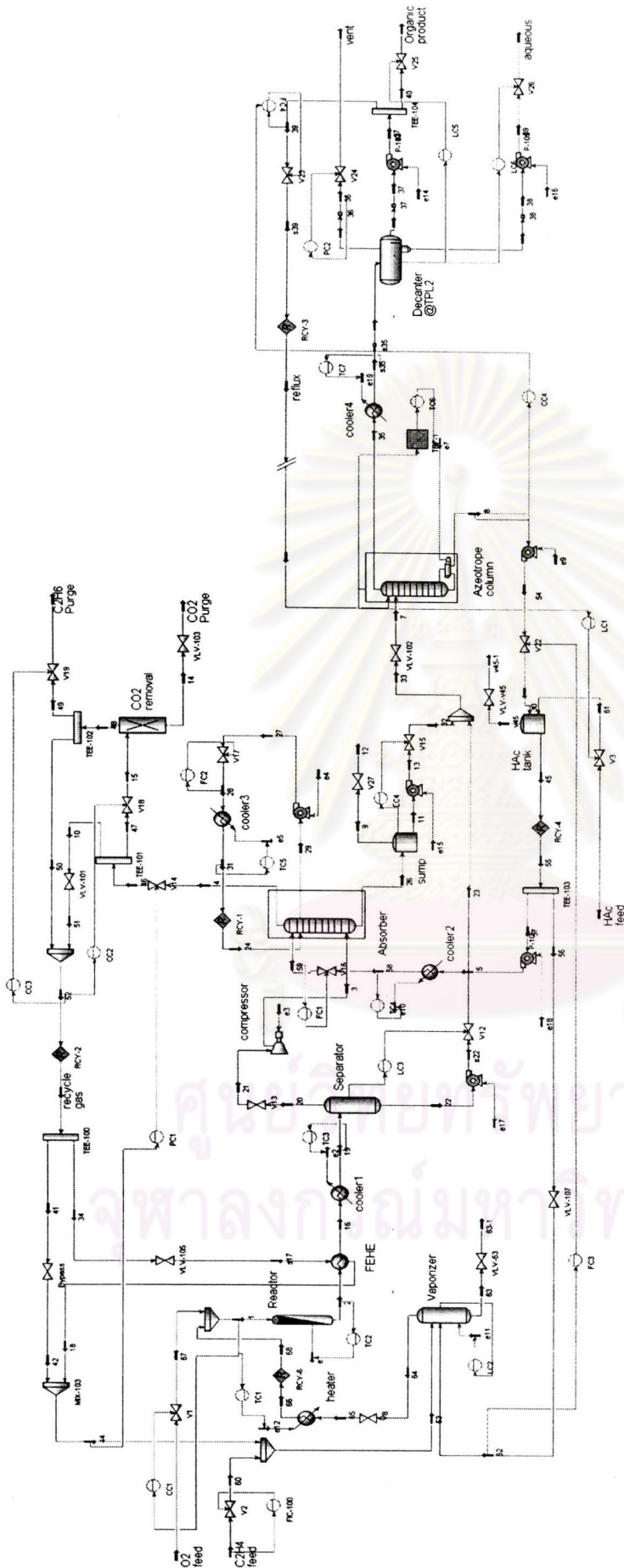


Figure A5 Designed control structure III (CS4) of Vinyl Acetate Process

APPENDIX B

Sizing Equipment

The steady state simulation does not need information that has no effect on steady state results. These items include column diameters, sizes of all surge vessels, sizes of control valves, etc. However, the dynamic simulation does need this information because the dynamic response of a process unit depends on the size of the equipment. The capacitance of the system (its time constant) is dictated by its size (volume or mass) relative to the flux (flowrate, heat-transfer rate, etc.). Therefore all equipment must be sized (at least approximately) before dynamic simulations can be performed.

Sizing equipment is necessary so that the dynamic capacitance of the equipment (tank sizes, column liquid holdups, heat-exchanger volumes, etc.) is available to the simulator. It is not necessary to have all the details of the mechanical design of the equipment. Some good estimates of the gas volumes and liquid holdups in a system are all that are necessary to predict realistic dynamic responses.

B1. Distillation Columns

The volume of a distillation column depends on its diameter D_c and length L_c . Both are easily calculated

- **Length:** A typical tray spacing is about two feet. So if the column has N_T trays, the height of the tray section is $2 N_T$ (feet). However, the column requires some additional height to accommodate reflux and feed entry locations and to provide surge volume in the base, particularly if therosiphon reboilers are used. Therefore we normally increase the length of the column by about 20%:

$$L_c (ft) = 2.4N_T$$

This approximation assumes that we are using actual trays. If the simulation uses theoretical trays, which is typically the case, an adjustment in the length should be made so that the actual volume of the vessel with real trays is used

$$L_c (ft) = 2.4(N_T)_{theoretical} / Efficiency$$

This use of theoretical trays also requires an adjustment in the weir height of the trays so that a realistic estimate of the total liquid holdup on the actual trays is used. Weir heights are normally one to two inches on actual trays. So the weir height specified in the simulation should be adjusted upwards by dividing by the efficiency.

Tray efficiency depends on several factors, but the most important is relative volatility or ease of separation. Components with large differences in boiling points (high relative volatilities) exhibit large changes in compositions from tray to tray in the column. This results in low tray efficiencies (vapor and liquid are not in phase equilibrium). Components with small differences in boiling points produce small changes in compositions from tray to tray, so efficiencies are high. In the absence of better data, some heuristics can be used to estimate efficiency. Relative volatilities around $\alpha = 1.1$ give almost 100% efficiency. Relative around $\alpha = 2$ give efficiencies in the 80% range. Relative volatilities around $\alpha = 4$ give efficiencies in the 80% range. These estimates can be used to adjust column heights and tray weir heights.

The liquid holdup (weir height) must also be adjusted if packing is used. One of the biggest differences between packing and trays is the smaller liquid holdup in packed towers. This makes the dynamic response of a packed column faster than a trayed column, which means that disturbance rejection is worse in packed columns than in columns with trays.

- **Diameter:** The diameter of a column is set by the maximum vapor velocity. This often occurs at the top of the column where the pressure is the lowest, which gives the lowest vapor density. However, if the feed is subcooled liquid, the maximum vapor rate can occur just below the feed tray because of the extra vapor needed to bring the feed up to the temperature of the feed tray. Changes in molar heats of vaporization, temperature and molecular weights can move the location of the worst-case tray location to other positions in the column. The steady-state simulator vapor profiles should be checked to find the tray with the maximum vapor velocity.

A simple way to calculate the maximum allowable vapor velocity is to use the "F-Factor" parameter.

$$F - Factor \equiv V_{\max} \sqrt{\rho_V}$$

In English Engineering units, the velocity V_{\max} has units of ft/sec and the vapor density has units of lb/ft³. In SI units, velocity is in m/sec and density is u

kg/m³. An F-Factor of 1 in English Engineering units or 1.22 in SI units can be used to determine the diameter of the column.

From the steady-state column profiles, select the tray with maximum vapor velocity from the given vapor flow rate and density.

B2. Separates (Flash Tanks)

Separates are tanks that have both liquid and vapor streams leaving the units. Their function is to disengage the two phases and provide liquid surge capacity. Therefore the vapor velocity must be kept low enough so that liquid entrainment is small. The F-Factor can be used to calculate the maximum diameter of the vessel. We use a more conservative F-Factor (0.5 in English Engineering units) so that effective separation of the two phases is achieved.

We also must check to see if the liquid holdup is adequate. The normal heuristic is to provide at least five minutes of holdup. This means the volume of liquid in the tank (normally with the interface at 50% of the tank height, assuming a vertical cylindrical vessel) should be five times the volumetric flowrate of the liquid leaving the tank.

To illustrate the calculations, we consider a flash tank operating at 48.9 °C (120°F) and 31.7 bar (460 psia). The vapor leaving the tank is 613 kg/hr (1251 lb/hr) with a vapor density of 46.3 kg/m³ (2.89 lb/ft³). The liquid leaving the tank is 1635 kg/hr (3604 lb/hr) with a liquid density of 460 kg/m³ (28.7 lb/ft³). The tank is a vertical cylindrical vessel with an aspect ratio (length-to-diameter ratio) of two

First we will calculate the required diameter based on the vapor velocity. The maximum vapor velocity, using a 0.5 F-Factor, is

$$V_{\max} = \frac{F - \text{Factor}}{\rho_v} = \frac{0.5}{\sqrt{2.89}} = 0.294 \text{ ft/sec}$$

The volumetric flowrate is (1251 lb/hr)(ft³ /2.89 lb)(hr/3600sec) = 0.130 ft³/sec. Therefore the cross-sectional area of the tank is

$$\text{Area} = \frac{0.294 \text{ ft}^3 / \text{sec}}{0.13 \text{ ft}^3 / \text{sec}} = 0.442 \text{ ft}^2$$

Thus the tank diameter must be at least [(4)(0.442)/π]^{0.5} = 0.75 feet.

Now we need to check the liquid holdup requirements. The volumetric flowrate of liquid is (3604 lb/hr)(ft³ /28.7 lb)(hr/60min) = 2.09 ft³/sec. To have 5

minutes holdup of liquid with the tank half full, the volume of the tank should be $(2)(5 \text{ min})(2.09 \text{ ft}^3/\text{min}) = 20.9 \text{ ft}^3$. With an aspect ratio of two, the relationship between volume and diameter is

$$Volume = \frac{\pi}{4} D^2 L = \frac{\pi}{4} D^2 (2D) = \frac{\pi}{2} D^3$$

Therefore the diameter is 2.37 ft. Since this is larger than that calculated from the vapor F-Factor, we specify a tank with a diameter of 2.5 ft and a length of 5 ft. Note that we have used vertical tanks in all the examples above. If horizontal tanks are used, the calculations must be modified to accommodate this change.

The dynamics of heaters and coolers (and column reboilers and condensers) are usually assumed to be fast compared to the composition and flow dynamics.

B3. Surge Volumes

Tanks and surge volumes are required whenever liquid is to be pumped. The reflux drum and the base (or reboiler) of a distillation column are examples. From a steady-state economic design point of view, capital investment is minimized by making these vessels as small as possible. However, from a dynamic point of view, we want to have lots of surge capacity so that disturbances in flowrates can be attenuated and we don't lose liquid levels.

The commonly used heuristic for surge vessel sizing is to provide about 5 minutes of liquid holdup with the vessel half full. This is based on the total flowrate of liquid into the vessel. If the liquid level is at 50% for the steady-state conditions, it will take 5 minutes to completely drain or fill the vessel if the inflow or outflow go to zero.

For example, suppose the total flow from a distillation column reflux drum (distillate plus reflux) is 5577 lb/hr with a liquid density of 29 lb/ft³. The size of the reflux drum should be

$$(5577 \text{ lb/hr})(\text{ft}^3 / 29 \text{ lb})(\text{hr}/60 \text{ min})(10 \text{ min}) = 32 \text{ ft}^3$$

To calculate drum diameter and length from the known volume, an aspect ratio (L/D) must be known. Aspect ratios of various vessels vary from 1 to 4, but for surge vessel a value of 2 is typical.

$$Volume = \frac{\pi}{4} D^2 L = \frac{\pi}{4} D^2 (2D) = \frac{\pi}{2} D^3$$

Surge volume is also used in decanters, which are vessels used to separate two liquid phases. The settling velocity of the droplets of the discontinuous heavy liquid phase in the continuous light phase depends on the density difference between the two phases. Large holdup times (20 to 30 minutes) are typically used in decanters to make sure there is good phase separation.

B4. Heat Exchangers

The volumes of both sides of the heat exchanger must be calculated if these contribute significant dynamics. For a tube-in-shell heat exchanger, these volumes can be quickly estimated from the known heat-transfer area that has been calculated in the steady-state simulation from the specified heat duty, overall heat-transfer coefficient and temperature differential driving force.

Let the known total heat-transfer area be A_{total} (in either m^2 or ft^2). Let the tube length be L and tube diameter D (m or ft). The circumferential heat-transfer area of each tube is

$$A_{tube} = \pi DL$$

The number of tubes required is

$$N_{tubes} = \frac{A_{total}}{A_{tube}} = \frac{A_{total}}{\pi DL}$$

The total volume inside all the tubes is

$$V_{tubes} = N_{tubes} \left(\frac{\pi D^2}{4} \right) L = \left(\frac{A_{total}}{\pi DL} \right) \left(\frac{\pi D^2}{4} \right) L = \left(\frac{D}{4} \right) A_{total}$$

Thus the calculation of the volume inside the tubes requires that we know the heat-transfer area and that we select a tube diameter.

$$V_{tubes} = \left(\frac{D}{4} \right) A_{total}$$

Typical tube diameters are 25 to 50 mm (1 to 2 inches).

For a numerical example, suppose the required heat-transfer area is 625 ft^2 and a tube diameter of 1 inch is selected. Then the tube volume is

$$V_{tubes} = \left(\frac{D}{4} \right) A_{total} = \left(\frac{1/12}{4} \right) 625 = 13 \text{ ft}^3$$

Now we need to calculate the volume of process material in the shell side. This is the total volume of the shell minus the volume of the tubes. The shell volume depends on the layout and spacing of the tubes, but at the conceptual design stage we do not need to go into all the nitty-gritty details. A simplifying approximation can be made that works pretty well for most tube-in-shell designs. We assume that the shell volume is equal to the tube volume.

$$V_{shell} \cong V_{tubes}$$

The approximate calculations discussed above are applicable to tube-in-shell heat exchangers. There are many other types of heat exchangers, and the appropriate sizes and holdups should be used for these units.



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APPENDIX C

Choosing the Correct Controller and Controller Tuning Parameters

C1. Choosing the Correct Controller

You should consider what type of performance criteria is required for the set point variables, and what acceptable limits they must operate within. Generally, an effective closed loop system is expected to be stable and cause the process variable to ultimately attain a value equal to the set point. The performance of the controller should be a reasonable compromise between performance and robustness. A very tightly tuned or aggressive controller gives good performance but is not robust to process changes. It could go unstable if the process changes too much. A very sluggishly tuned controller delivers poor performance but will be very robust. It is likely to become unstable. The following is a flowchart that outlines a method for choosing a feedback controller in figure C1.

In general, if offset can be tolerated, a proportional controller should be used. If there is significant noise, or if there is significant dead time and/or a small capacity in the process, the PI controller should be used. If there is no significant noise in the process, and the capacity of the system is large and there is no dead time, a PID controller may be appropriate. It is apparent why the PI controller is the most common controller found in a plant. There are three possible conditions that a PI controller can handle, whereas the PID controller requires a specific set of conditions in order to be used effectively.

C2. Choosing Controller Tuning Parameters

The following is a list of general tuning parameters appropriate for various processes. The suggested controller settings are optimized for a quarter decay ratio error criterion. Keep in mind that there is no single correct way of tuning a controller.

The objective of control is to provide a reasonable compromise between performance and robustness in the closed loop response. The following rules are approximate. They will provide you very close to tight control. You can adjust the tuning parameters further if the closed loop response is not satisfactory. Tighter control and better performance can be achieved by increasing the gain. Decreasing the controller gain results in a slower but more stable response. Generally, proportional control can be considered the principal controller. Integral and derivative action should be used to trim the proportional response. Therefore, the controller gain should be tuned first with the integral and derivative actions set to a minimum. If instability occurs, the controller gain should be adjusted first. Adjustments to the controller gain should be made gradually.

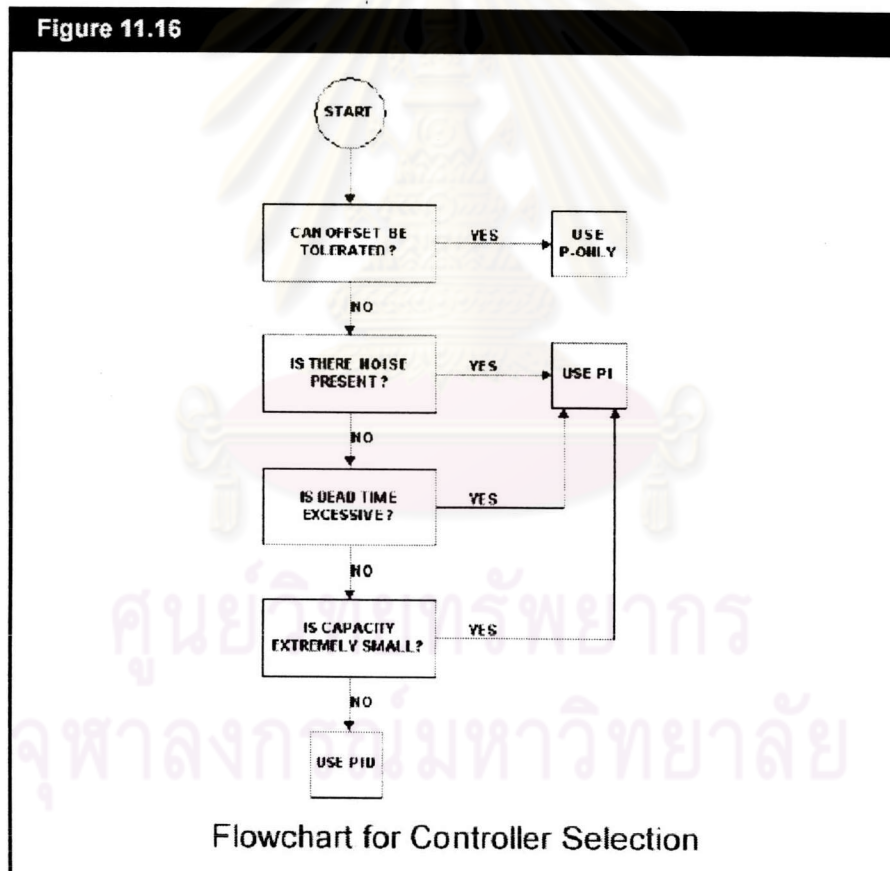


Figure C1 Flowchart that outlines a method for choosing a feedback controller

Flow Control

Flow in a pipe is typically a very fast responding process. The dead time and capacity associated with a length of pipe is generally very small. It is therefore not unusual for the process to be limited by the final control element (valve) dynamics. You can easily incorporate valve dynamics in the HYSYS model by modifying the valve parameters in the Actuator page of the Dynamics tab. Tuning a flow loop for PI control is a relatively easy task. In order for the flow measurement to track the setpoint very closely, the gain, K_c , should be set between 0.4 and 0.65 and the integral time, T_i , should be set between 0.05 and 0.25 minutes. Since the flow control is fast responding, it can be used effectively as the secondary controller in a cascade control structure. The non-linearity in the control loop may cause the control loop to become unstable at different operating conditions. Therefore, the highest process gain should be used to tune the controller. If a stability limit is reached, the gain should be decreased, but the integral action should not. Since flow measurement is naturally noisy, derivative action is not recommended.

Liquid Pressure Control

Like the flow loop process, the liquid pressure loop is typically very fast. The process is essentially identical to the liquid flow process except that liquid pressure instead of flow is controlled using the final control element. The liquid pressure loop can be tuned for PI and Integral-only control, depending on your performance requirements. Like flow control, the highest process gain should be used to tune the controller. Typically, the process gain for pressure is smaller than the flow process gain. The controller gain, K_c , should be set between 0.5 and 2 and the integral time, T_i , should be set between 0.1 and 0.25 minutes.

Liquid Level Control

Liquid level control is essentially a single dominant capacity without dead time. In some cases, level control is used on processes which are used to attenuate disturbances in the process. In this case, liquid level control is not as important. Such processes can be controlled with a loosely tuned P-only controller. If a liquid level offset cannot be tolerated, PI level controllers should be used. There is some noise associated with the measurement of level in liquid control. If this noise can be

practically minimized, then derivative action can be applied to the controller. It is recommended that K_c be specified as 2 and the bias term, OP_{ss} , be specified as 50% for P-only control. This ensures that the control valve is wide open for a level of 75% and completely shut when the level is 25% for a setpoint level of 50%. If PI control is desired, the liquid level controller is typically set to have a gain, K_c , between 2 and 10. The integral time, T_i , should be set between 1 and 5 minutes. Common sense dictates that the manipulated variable for level control should be the stream with the most direct impact on the level. For example, in a column with a reflux ratio of 100, there are 101 units of vapor entering the condenser and 100 units of reflux leaving the reflux drum for every unit of distillate leaving. It makes sense that the reflux flow or vapor boilup be used to control the level of the reflux drum. If the distillate flow is used, it would only take a change of slightly more than 1% in either the reflux or vapor flow to cause the controller to saturate the distillate valve.

Gas Pressure Control

Gas pressure control is similar to the liquid level process in that it is capacity dominated without dead time. Varying the flow into or out of a vessel controls the vessel pressure. Because of the capacitive nature of most vessels, the gas pressure process usually has a small process gain and a slow response. Consequently, a high controller gain can be implemented with little chance of instability. The pressure loop can easily be tuned for PI control. The controller gain, K_c , should be set between 2 and 10 and the integral time, T_i , should be set between 2 and 10 minutes. Like liquid level control, it is necessary to determine what affects pressure the most. For instance, on a column with a partial condenser, you can determine whether removing the vapor stream affects pressure more than condensing the reflux. If the column contains noncondensables, these components can affect the pressure considerably. In this situation, the vent flow, however small, should be used for pressure control.

Temperature Control

Temperature dynamic responses are generally slow, so PID control is used. Typically, the controller gain, K_c , should be set between 2 and 10, the integral time, T_i , should be set between 2 and 10 minutes, and the derivative time T_d , should be set between 0 and 5 minutes.

VITA

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