

CHAPTER 2: CASE STUDIES

2.1 INTRODUCTION

In this chapter, the modeling of the basic case studies (representing the heart of the chemical engineering industry) is undertaken. Tutorials and exercises that can be carried out upon these case studies will be discussed in other chapters. These modules (case studies) are clearly defined and all involved parameters are explained. It is important to understand the mathematical development of the models as they represent the basis to which the exercises will be referred to. The mathematical models developed here for each case study are core to the process transfer functions that will be used with differing controller algorithms and are classical examples from literature.

As listed earlier, these case studies are;

1. Forced-Circulation Evaporator
2. Polyethylene Reactor
3. Waste Water Treatment Unit
4. Ethylene Dimerization Process
5. Double Effect Evaporator
6. Two-CSTR in Series
7. Multi-Stage Flash Desalination Plant

2.2 FORCED-CIRCULATION EVAPORTOR UNIT

2.2.1 Process Description and Flow sheet

The forced-circulation evaporator is a common processing unit in sugar mills, alumina production and paper manufacture. This process is used to concentrate a dilute liquor by evaporating its solvent (usually water) as shown in the Fig. 2.1.

A feed stream with solute of concentration C_1 (mass percentage) is mixed with high volumetric recycle flow rate and fed to a vertical evaporator (heat exchanger). The solution will pass through the tube. A saturated steam is used to heat up the mixture by condensing on the outer surface of the tubes. The liquor which passes up inside the tube boils and then passes to a separator vessel. In the separator, the liquid and vapor are separated at constant temperature and pressure. The liquid is recycled with some being

drawn off as product with solute concentration of C_2 . The vapor is usually condensed with water. Water is used as the coolant.

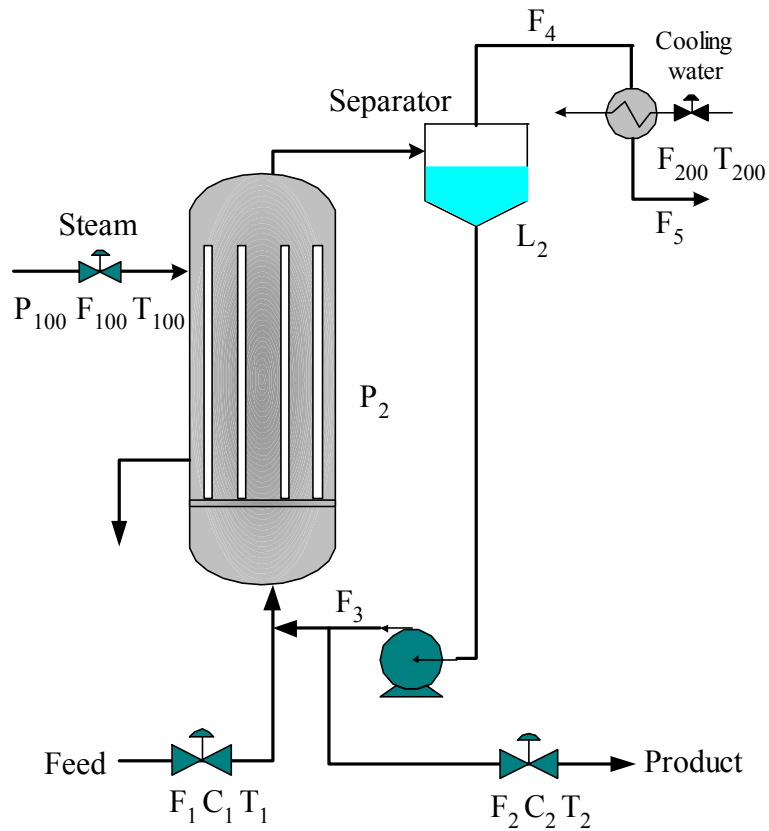


Fig. 2.1 Flow sheet of Forced Circulation Evaporator Process

2.2.2 The Process Model

$$\rho A \frac{dL_2}{dt} = F_1 - F_4 - F_2 \quad (2.1)$$

$$M \frac{dC_2}{dt} = F_1 C_1 - F_2 C_2 \quad (2.2)$$

$$W \frac{dP_2}{dt} = F_4 - F_5 \quad (2.3)$$

Additional relations:

$$T_2 = 0.5616P_2 + 0.3126C_2 + 48.43 \quad (2.4)$$

$$T_3 = 0.507P_2 + 55.0 \quad (2.5)$$

$$F_2 = F_1 - F_4 \quad (2.6)$$

$$F_4 = [Q_{100} - F_1 Cp(T_2 - T_1)]/\lambda \quad (2.7)$$

$$T_{100} = 0.1538P_{100} + 90.0 \quad (2.8)$$

$$Q_{100} = F_{100}\lambda_s = UA_1(T_{100} - T_2) \quad (2.9)$$

$$Q_{200} = F_{200}Cp(T_{201} - T_{200}) = UA_2(T_3 - 0.5*(T_{200} + T_{201})) \quad (2.10)$$

$$F_5 = Q_{200}\lambda \quad (2.11)$$

$$UA_1 = 0.16(F_1 + F_3) \quad (2.12)$$

2.2.3 Process Parameters and Variables

<i>Variable</i>	<i>Description</i>	<i>Value</i>	<i>Units</i>
F ₁	Feed flow rate	10.0	kg/min
F ₂	Product flow rate	2.0	kg/min
F ₃	Circulating flow rate	50.0	kg/min
F ₄	Vapor flow rate	8.0	kg/min
F ₅	Condensate flow rate	8.0	kg/min
C ₁	Feed composition	5.0	Percent
C ₂	Product composition	25.0	Percent
T ₁	Feed temperature	40.0	C
T ₂	Product temperature	84.6	C
T ₃	Vapor temperature	80.6	C
L ₂	Separator level	1.0	m
P ₂	Operating pressure	50.5	kPa
F ₁₀₀	Steam flow rate	9.3	kg/min
T ₁₀₀	Steam temperature	119.9	C
P ₁₀₀	Steam pressure	194.7	kPa
Q ₁₀₀	Heater duty	339.0	kW
F ₂₀₀	Cooling water flow rate	208.0	Kg/min
T ₂₀₀	Cooling water inlet temperature	25.0	C
T ₂₀₁	Cooling water outlet temperature	46.1	C
Q ₂₀₀	Condenser duty	307.9	kW
ρ _A	Mass holdup in the separator	20	kg/m

M	Solute holdup	20	kg
W	Constant	4	kg/kPa
λ	Latent heat of vaporization of water	38.5	kW/kg
UA ₂	Heat transfer coefficient times the heat transfer area	6.84	kW/K

λ_s is the latent heat of steam which is calculated from a given correlation as a function of the saturation temperature.

2.3.2 The Process Model

$$V_g \frac{dC_{M1}}{dt} = F_{M1} - x_{M1}B_t - R_{M1} \quad (2.13)$$

$$V_g \frac{dC_{M2}}{dt} = F_{M2} - x_{M2}B_t - R_{M2} \quad (2.14)$$

$$V_g \frac{dC_H}{dt} = F_H - x_H B_t - R_H \quad (2.15)$$

$$V_g \frac{dC_N}{dt} = F_N - x_N B_t \quad (2.16)$$

$$\frac{dY_c}{dt} = F_c a_c - k_d Y_c - O_p Y_c / B_w \quad (2.17)$$

$$(M_r C_{p_r} + B_w C_{p_p}) \frac{dT}{dt} = HF + HG - HR - HT - HP \quad (2.18)$$

$$M_g C_{p_g} \frac{dT_g}{dt} = F_g C_{p_g} (T_{gi} - T_g) + F_w C_{p_w} (T_{wi} - T_{wo}) \quad (2.19)$$

$$P_t = (C_{M1} + C_{M2} + C_H + C_N)RT \quad (2.20)$$

$$T_{gi} = \left(\frac{P_t}{P_t + \Delta P} \right)^{(1-\eta)/\eta} T \quad (2.21)$$

$$F_w C_{p_w} (T_{wi} - T_{wo}) = 0.5UA[(T_{wo} + T_{wi}) - (T_{gi} + T_g)] \quad (2.22)$$

$$HF = (F_{M1} C_{p_{M1}} + F_{M2} C_{p_{M2}} + F_H C_{p_H} + F_N C_{p_N})(T_f - T_{ref}) \quad (2.23)$$

$$HG = F_g C_{p_g} (T_g - T_{ref}) \quad (2.24)$$

$$HT = (F_g + B_t) C_{p_g} (T - T_{ref}) \quad (2.25)$$

$$HP = O_p C_{p_p} (T - T_{ref}) \quad (2.26)$$

$$HR = M_{w1} R_{M1} \Delta H_r \quad (2.27)$$

$$O_p = M_{w1} R_{M1} + M_{w2} R_{M2} \quad (2.28)$$

$$R_{M1} = C_{M1} Y_c k_{p1} e^{-\frac{E}{R}(1/T - 1/T_{ref})} \quad (2.29)$$

$$R_{M2} = C_{M2} Y_c k_{p2} e^{-\frac{E}{R}(1/T - 1/T_{ref})} \quad (2.30)$$

$$C_{p_g} = \sum x_i C_{p_i} \quad (2.31)$$

2.3.3 Process Parameters and Variables

<i>Variable</i>	<i>Description</i>	<i>Value</i>	<i>Units</i>
a_c	Active site concentration	0.548	mole/kg
B_w	Mass of the polymer in the bed	70.0	tonne
B_t	Bleed flow rate	10.39	mole/s
C_{M1}	Concentration of monomer,	297.06	mole/m ³
C_{M2}	Concentration of co-monomer	116.17	mole/m ³
C_N	Concentration nitrogen	166.23	mole/m ³
C_H	Concentration of hydrogen	105.78	mole/m ³
C_{pM1}	Heat capacity of monomer	11	cal/mole K
C_{pM2}	Heat capacity of co-monomer	24	cal/mole K
C_{pH}	Heat capacity of hydrogen	7.7	cal/mole K
C_{pN}	Heat capacity of nitrogen,	6.9	cal/mole K
C_{pw}	Heat capacity of recycle gas and water	18.0	cal/mole K
C_{pp}	Heat capacity of polymer,	0.85	cal/g K
E	Activation energy for propagation,	9000	cal/mole
F_c	Catalyst flow rate	2.0	kg/s
F_w	Cooling water flow rate,	5.6×10^5	mole/s
F_g	recycle flow rate,	8500	mole/s
F_{M1}	Monomer flow rate,	131.13	mole/s
F_{M2}	co-monomer flow rate,	3.51	mole/s
F_N	hydrogen flow rate,	1.6	mole/s
F_H	nitrogen flow rate,	2.52	mole/s
k_d	Deactivation rate constant,	0.0	1/s
k_{p1}	Propagation rate constant for monomer	85.0	L/mole s
k_{p2}	Propagation rate constant for co-monomer,	3.0	L/mole s
M_w	Water holdup in the heat exchanger,	2×10^6	mole
$M_r C_{p_r}$	Thermal capacitance of the reaction vessel,	14×10^6	kcal/K
Op	Polymer outlet rate,	3.6434	kg/s
P_t	Total pressure,	20.0	atm
P_{M1}	Partial pressure of monomer	8.67	atm
P_{M2}	Partial pressure of co-monomer	3.39	atm
P_N	Partial pressure of nitrogen	4.8525	atm
P_H	Partial pressure of hydrogen,	3.0875	atm

R	Ideal Gas constant,	82.6×10^{-6}	atm m ³ /K mole
T	Bed temperature,	82	°C
T_f	feed temperature,	25	°C
T_{ref}	reference temperature,	87	°C
T_{gi}	Temperature of recycle stream before cooling	136	°C
T_g	Temperature of recycle stream after cooling,	51.7	°C
T_{wi}	Cooling water temperature before cooling,	20	°C
T_{wo}	Cooling water temperature after cooling,	35	°C
Y_c	Number of moles of catalyst site, mole	5.849	mole
ΔH_r	Heat of reaction	-894	cal/g

The system has two internal (built-in) PI control loops which are set as:

Control loop	k_c	τ_I
Pt \rightarrow Bt	10	10
T \rightarrow Tw	3	20

2.4 ETHYLENE DIMERIZATION REACTOR

2.4.1 Process Description and Flow Sheet

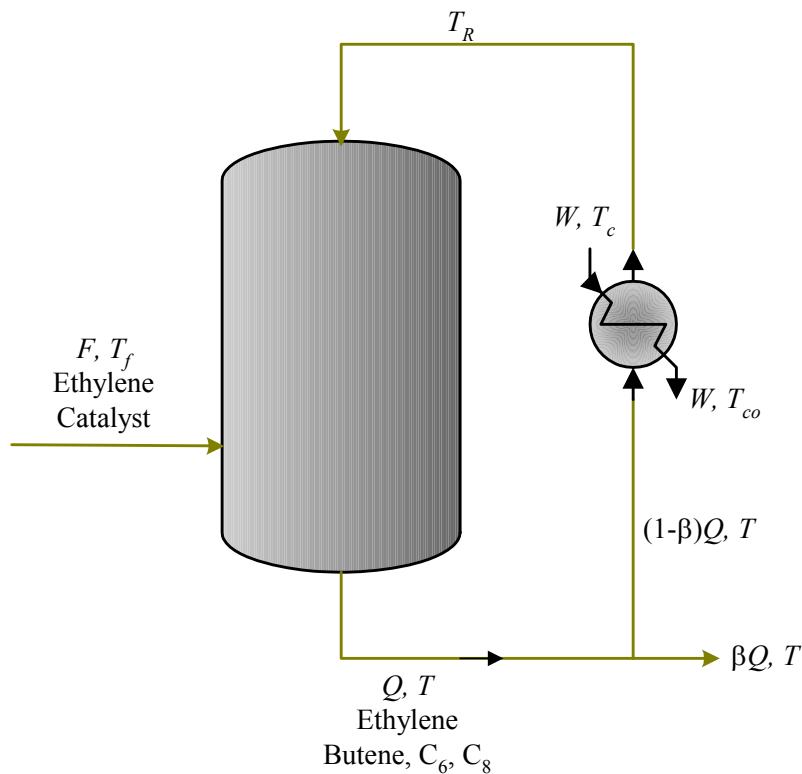


Fig. 2.3 Dimerization Reactor

The catalytic dimerization of ethylene is considered to be one of the most promising methods for producing butene-1, the first member of the even-numbered linear 1-alkenes which have diversified applications. This process uses a homogeneous titanium-based catalyst which demonstrates high dimerization activity coupled with excellent selectivity to butene-1 at moderate pressure (20-30 psia) and temperature (50-60 °C). The dimerization reaction is regarded as a degenerate ethylene polymerization reaction and therefore the formation of heavier oligomers is expected. The industrial ethylene dimerization reactor is operating in liquid phase at bubble point conditions. Fresh ethylene and homogeneous catalyst are fed continuously to the reactor where the exothermic reaction is removed by means of external loop equipped with a cooler.

The dimerization reactor considered in this study is assumed to be a liquid phase perfectly mixed reactor, i.e. no mass transfer limitation is considered in this system. Schematic of the process is depicted in Fig. 2.3. The liquid is homogenized by a high recirculation rate around the reactor through a heat exchange used to remove the high

exothermic heat of reaction. The model uses the Homo- and Co-polymerization mechanisms suggested by Galtier *et. al.* [9]. The reaction stages; initiation, propagation and termination are of first order kinetics with respect to each reactant.

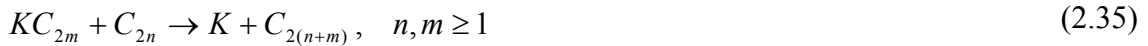
Initiation and propagation stages:



The rate of initiation and propagation, which also represent the rate of disappearance of C_{2n} in these stages, have the following rate equation:

$$r_{a_{2n}} = a_{2n} [C_{2n}] \sum_{m=0}^{\infty} [KC_{2m}] \quad (2.34)$$

Termination stage:



The chain termination reactions, which are assumed to occur in parallel with the growth reactions have the following rate equations:

$$r_{b_{2n}} = b_{2n} [C_{2n}] \sum_{m=1}^{\infty} [KC_{2m}] \quad (2.36)$$

The rate constants are defined as follows:

$$a_2 = a_{20} e^{-E_1 \left(\frac{1}{T} - \frac{1}{T_r} \right)} \quad (2.37)$$

$$a_4 = a_{40} e^{-E_1 \left(\frac{1}{T} - \frac{1}{T_r} \right)} \quad (2.38)$$

$$b_4 = a_{40} e^{-E_1 \left(\frac{1}{T} - \frac{1}{T_r} \right)} \quad (2.39)$$

$$b_2 = b_{20} a_2 e^{-E_2 \left(\frac{1}{T} - \frac{1}{T_r} \right)} \quad (2.40)$$

Based on the above assumptions and the assumed reaction kinetics, the resulted dynamic model of the dimerization process is presented in the following [1],[6].

2.4.2 The Process Model

$$V \frac{dC_4}{dt} = -Q\beta C_4 - V[(-b_2C_2 + a_4C_4 + b_4C_4)K_2 + a_4C_4K + b_4C_4K_4] \quad (2.41)$$

$$V \frac{dC_2}{dt} = FC_{2f} - Q\beta C_2 - V[a_2C_2(K + K_2 + K_4) + b_2C_2(K_2 + K_4 + K_6)] \quad (2.42)$$

$$V \frac{dC_6}{dt} = -FC_6 + V[b_4C_4K_2 + b_2C_2K_4] \quad (2.43)$$

$$V \frac{dC_8}{dt} = -FC_8 + V[b_4C_4K_4 + b_2C_2K_6] \quad (2.44)$$

$$V \frac{dK}{dt} = FK_f - Q\beta K - V[(a_2C_2 + a_4C_4)K + b_2C_2(K_2 + K_4 + K_6) + b_4C_4(K_2 + K_4)] \quad (2.45)$$

$$V\rho C_p \frac{dT}{dt} = F\rho_f C_{pf}(T_f - T_r) + Q(1 - \beta)\rho C_p(T_R - T_r) - Q\rho C_p(T - T_r) + V(r_2(-\Delta H_1) + r_4(-\Delta H_2)) \quad (2.46)$$

$$V_c \rho C_p \frac{dT_R}{dt} = Q(1 - \beta)\rho C_p(T - T_R) - UA(T_{Rav} - T_{cav}) \quad (2.47)$$

$$V \frac{dK_2}{dt} = -Q\beta K_2 + V[a_2C_2K - (a_2C_2 + a_4C_4 + b_2C_2 + b_4C_4)K_2] \quad (2.48)$$

$$V \frac{dK_4}{dt} = -Q\beta K_4 + V[a_2C_2K_2 - (a_2C_2 + b_2C_2 + b_4C_4)K_4 + a_4C_4K] \quad (2.49)$$

$$V \frac{dK_6}{dt} = -Q\beta K_6 + V[a_2C_2K_4 - b_2C_2K_6 + a_4C_4K_2] \quad (2.50)$$

where

$$T_{Rav} = \frac{T + T_R}{2} \quad (2.51)$$

$$T_{cav} = \frac{T_c + T_{co}}{2} \quad (2.52)$$

The dynamic of the outlet temperature of the coolant fluid is not included and alternatively it is obtained by solving the steady-state equation:

$$WC_p(T_{co} - T_c) = U_h A_c (T_{Rav} - T_{cav}) \quad (2.53)$$

2.4.3 Process Parameters and Variables

Variable	Description	Value	Units
a_2	Rate constant for consumption of component C_2 in the initiation and propagation		$(m^3/mole \cdot s)$.

a_4	Rate constant for consumption of component C_4 in the initiation and propagation	$(m^3/mole\ s)$.
b_2	Rate constant for consumption of component C_2 in the termination stage	$(m^3/mole\ s)$.
b_4	Rate constant for consumption of component C_4 in the termination stage	$(m^3/mole\ s)$.
C_p	Heat capacity of reactor mixture	0.55 $(cal/gm, ^\circ C)$
C_{p_f}	Heat capacity of feed	0.55 $(cal/gm, ^\circ C)$
C_{p_w}	Heat capacity of water	1.0 $(cal/gm, ^\circ C)$
C_4	Butene-1 concentrations,	8700 $(mole/m^3)$
C_2	ethylene concentrations,	1065 $(mole/m^3)$
C_{2f}	Ethylene concentration at the feed	25000 $(mole/m^3)$
E_1	Activation energy for initiation & propagation reactions	-6000 K
E_2	Activation energy for the termination reaction	3000 K
F	Reactor fresh feed	0.004 (m^3/s)
K	Catalyst	1.122 $(mole/m^3)$
K_2	Catalyst activator for C_2	0.1345 $(mole/m^3)$
K_4	catalyst activator for C_4	0.0178 $(mole/m^3)$
K_6	Catalyst activator for C_6	0.0028 $(mole/m^3)$
K_f	Catalyst concentration at the fresh feed	1.25 $(mole/m^3)$
Q	Product flow rate	F/β (m^3/s)
T_c	Inlet coolant temperature	0.0 $(^\circ C)$
T_f	Feed temperature	30.0 $(^\circ C)$
T_r	Reference temperature	25.0 $(^\circ C)$
T	Reactor temperature	67.0 $(^\circ C)$
T_R	Recycle temperature	43.0 $(^\circ C)$
$U_h A_c$	Heat transfer coefficient times heat transfer area	27500 $(cal\ s\ ^\circ C)$
V	Reactor volume (m^3)	500 m^3
V_c	Cooler volume	50 m^3
W	Coolant flow rate,	500 (kg/s)
ρ	Mixture density	500 Kg/m^3
ΔH_{ri}	Heat of reaction	25000 $Cal/mole$
β	Recycle ratio	0.02

2.5 DOUBLE EFFECT EVAPORATOR

2.5.1 Process Description and Flow Sheet

A schematic flow sheet of the process is shown in Fig. 2.4. A solution of triethylene glycol in water is fed to the first effect at flow rate F , solute concentration C_f , and temperature T_f . The solution is concentrated in the first effect using steam at flow rate W_s , generating the overhead vapor stream O_1 and the concentrated bottom stream B_1 with solute concentration C_1 . The bottom stream B_1 is fed to the tube side of the second

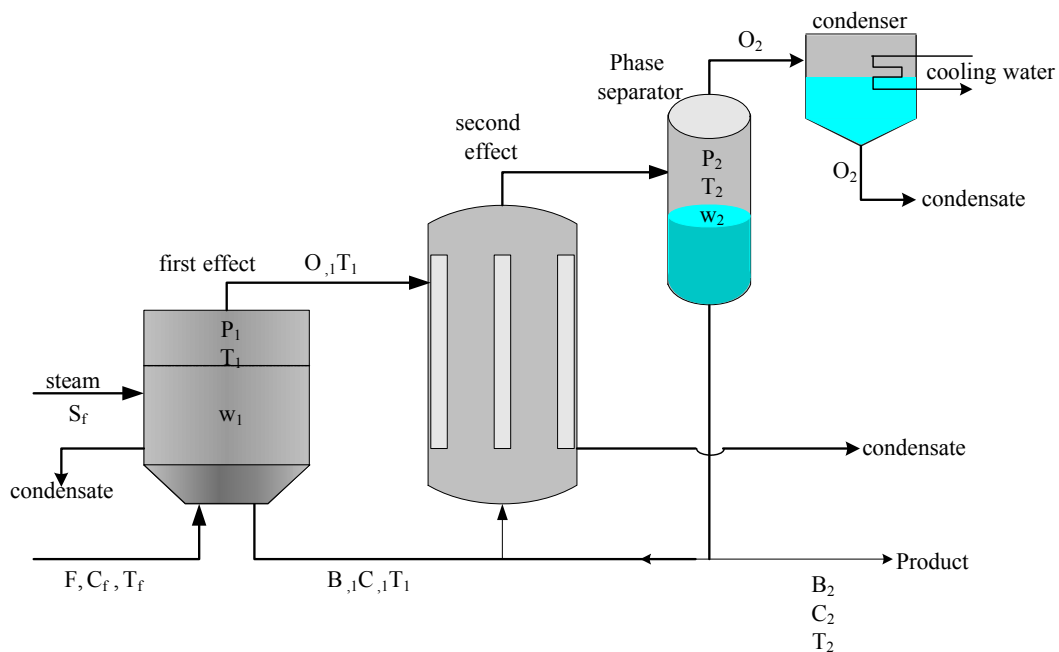


Fig. 2.4 Two Effect Evaporator

effect at a lower pressure, while the overhead stream O_1 is fed to the shell side. The bottom stream B_2 , which is the product stream, leaves the second effect with solute concentration C_2 . The overhead stream O_2 from the second effect is condensed and released as condensate. W_1 and W_2 are the liquid holdups, whereas P_1, T_1 and P_2, T_2 are the pressures and temperatures in the first and second effects, respectively.

A standard modeling procedure was followed to develop a dynamic model for the process using the following assumptions:

1. The steam chests, tube walls and so on have negligible heat capacity.
2. The temperature T_2 is held constant by pressure controller.

3. The overhead vapor streams leaving each of the effects have negligible solute concentration compared to the respective bottom liquid streams.
4. Vapor holdup in each effect is negligible.

Here, assumption 2 is relaxed. The stream O_2 is fixed and the temperature T_2 is evaluated such that it respects the algebraic energy balance on the second effect. In the original model, O_1 is determined from the energy balance on the first effect. Here, O_1 is determined from the pressure difference between the two effects. In addition, the bottom streams B_1 and B_2 are used to control the liquid holdups W_1 and W_2 .

2.5.2 The Process Model

$$\frac{dW_1}{dt} = F - B_1 - O_1 \quad (2.54)$$

$$W_1 \frac{dC_1}{dt} = F(C_f - C_1) - O_1 C_1 \quad (2.55)$$

$$W_1 \frac{dh_1}{dt} = F(h_f - h_1) - O_1(H_{v1} - h_1) + Q_1 - L_1 \quad (2.56)$$

$$\frac{dW_2}{dt} = B_1 - B_2 - O_2 \quad (2.57)$$

$$W_2 \frac{dC_2}{dt} = B_1(C_1 - C_2) - O_2 C_2 \quad (2.58)$$

$$O_2(H_{v2} - h_2 + \frac{\partial h_2}{\partial C_2} C_2) = B_1(h_1 - h_2) + Q_2 - L_2 + \frac{\partial h_2}{\partial C_2} B_1(C_2 - C_1) \quad (2.59)$$

Additional relations:

$$h_i = f(T_i) \quad (2.60)$$

$$H_i = f(T_i) \quad (2.61)$$

$$Q_1 = U_1 A_1 (T_{s1} - T_1) = W_s \lambda \quad (2.62)$$

$$Q_2 = U_2 A_2 (T_1 - T_2) \quad (2.63)$$

$$L_1 = h_{w1} A_1 (T_w - T_1) \quad (2.64)$$

$$L_2 = h_{w2} A_2 (T_w - T_2) \quad (2.65)$$

$$O_1 = k_v \sqrt{(P_1 - P_2)} \quad (2.66)$$

$$P_1 = f(T_1) \quad (2.67)$$

$$P_2 = f(T_2) \quad (2.68)$$

Level Controllers:

$$B_1 = B_{1i} + k_{c1}(r_1 - W_1) \quad (2.69)$$

$$B_2 = B_{2i} + k_{c2}(r_2 - W_2) \quad (2.70)$$

Notes:

The current model is different than the original one in the following aspects:

- The overhead flow out of the first effect is defined in the original model by the heat transfer equation, which can be calculated as the amount vaporized at the given temperature of the first effect. In this model it is defined by the pressure difference between the two effects, i.e. (2.66).
- The overhead flow out of the second effect is defined in the original model by the heat balance equation around the second effect (2.59). In this model it is defined as manipulated variable.
- The temperature of the second effect is fixed in the original model. Here it is given by (2.59) after modification as follows:

$$W_2 \frac{dh_2}{dt} = -O_2 (H_{v2} - h_2 + \frac{\partial h_2}{\partial C_2} C_2) + B_1 (h_1 - h_2) + Q_2 - L_2 + \frac{\partial h_2}{\partial C_2} B_1 (C_2 - C_1)$$

- The specific enthalpy of Equation 2.60 & 2.61 are determined from an empirical correlations developed by the author of the original model. Here, common enthalpy correlations for water are used.
- In the current model, water vapor pressure correlations are included in order to calculate the vapor flow rate in (2.66).
- The proportional controllers, (2.69 & 2.70) are used here where indicated to control the liquid level in the corresponding effects.

- The sensitivity of the enthalpy of the solution $\frac{\partial h}{\partial c}$ is given by empirical relation in the original model. Here, it is estimated from enthalpy correlation for brine.

2.5.3 Process Parameters and Variables

<i>Variable</i>	<i>Description</i>	<i>Value</i>	<i>Units</i>
A ₁	Heat transfer area of 1 st effect		ft ²
A ₂	Heat transfer area of 2 ^{ed} effect	4.6	ft ²
B ₁	Bottom stream of 1 st effect	3.315	lb/min
B ₂	Bottom stream of 2 ^{ed} effect	1.715	lb/min
C ₁	Solute concentration in 1 st effect	4.8262	Wt%
C ₂	Solute concentration in 2 ^{ed} effect	9.3307	Wt%
C _f	Solute concentration in the feed	3.2	Wt%
F	Feed flow rate	5	lb/min
h _f	Enthalpy of the feed		Btu/lb
h _i	Liquid enthalpy in the i th effect		Btu/lb
H _i	Vapor enthalpy in the i th effect		Btu/lb
h _{wi}	Heat transfer coefficient in the i th effect	0	Btu/minF ft ²
k _v	Valve coefficient	1.7824	
L ₁	Heat loss in the 1 st effect	0	Btu/lb
L ₂	Heat loss in the 2 ^{ed} effect	0	Btu/lb
O ₁	Overhead stream of the 1 st effect	1.7	Lb/min
O ₂	Overhead stream of the 2 ^{ed} effect	1.6	Lb/min
P ₁	Operating pressure in the 1 st effect	25	psi
P ₂	Operating pressure in the 2 ^{ed} effect	7.5	psi
T ₁	Temperature in the 1 st effect	225	°F
T ₂	Temperature in the 2 ^{ed} effect	160	°F
T _f	Feed temperature	190	°F
T _w	Wall temperature	77	°F
U	Heat transfer coefficient	5.2345	Btu/minF ft ²
W ₁	Liquid holdup in the 1 st effect	30	Lb
W ₂	Liquid holdup in the 2 ^{ed} effect	35	Lb
λ	Latent heat of vaporization of water	948	Btu/lb

2.6 MULTI-STAGE FLASH DESALINATION

2.6.1 Process Description and Flow Sheet

In a typical MSF plant shown in Fig. 2.5 we can distinguish between three basic sections: heat rejection section, heat recovery section and the brine heater. On leaving the first (warmest) rejection stage the feed stream is split into two parts, reject sea water which passes back to the sea and a make up stream, which is then recycled back to the flash section of the last stage. A recycle stream, which is drawn from the last stage, passes through a series of heat exchangers, its temperature rises as it proceeds towards the heat input section of the plant. Passing through the brine heater the brine temperature is raised from the feed temperature at the inlet of the brine heater to a maximum value approximately equals to the saturation temperature at the system pressure. The brine then enters the first heat recovery stage through an orifice thus reducing the pressure. As the brine was already at its saturation temperature it will become superheated for a lower pressure and flashes to give off water vapor. The vapor then passes through a wire mesh (demister) to remove any entrainment brine droplets and onto a heat exchanger where the vapor is condensed and drips into a distillate tray. The process is then repeated all the way through the plant as both brine and distillate enter the next stage which is at a lower pressure. The concentrated brine is divided into two parts as it leaves the plant, a blow-down, which is pumped back to the sea and the recycle stream.

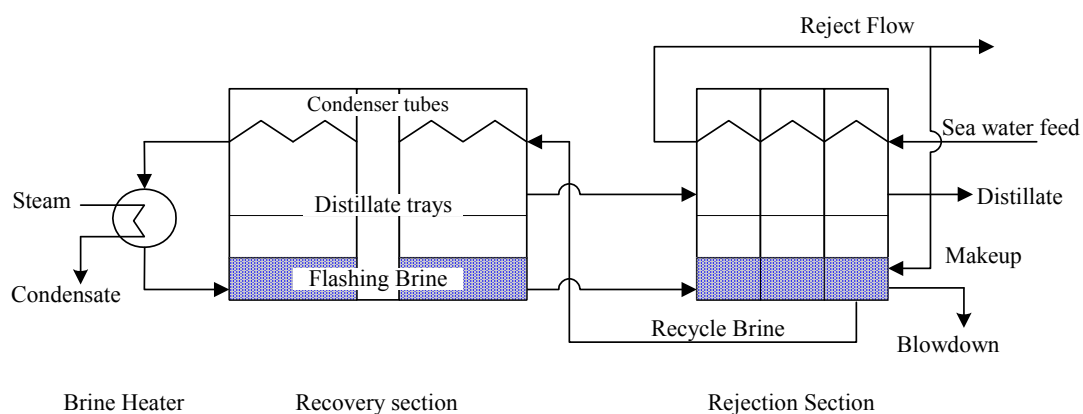


Fig. 2.5 Flow Sheet for the MSF process

2.6.2 The Process Model

The design and analysis of process operation requires the use of a rigorous model of the MSF plant. A first principle model for a 22 stages MSF plant was developed and validated [2]. The specific plant consists of 3 rejection section stages and 19 recover section stages. In the

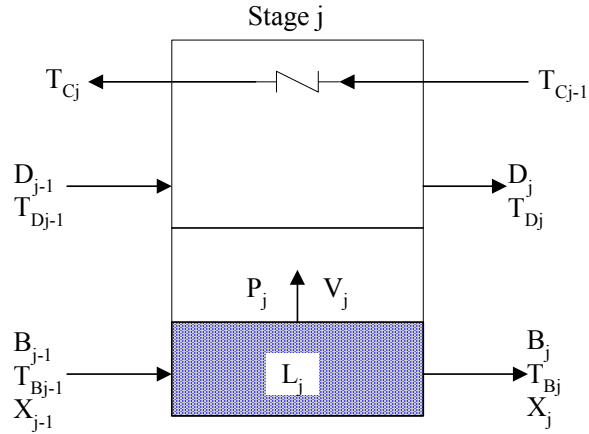


Fig. 2.5b Single Stage

following a summary of the developed model is given. Each plant stage is shown in Fig. 2.5b. The process is therefore defined by nine variables: brine pool height (L_j), brine flow rate (B_j), salt mass fraction (X_j), brine temperature (T_{Bj}), distillate flow rate (D_j), distillate temperature (T_{Dj}), coolant temperature (T_{Cj}), vaporization rate (V_j) and stage pressure (P_j). Furthermore and in order to minimize the size of the model the liquid levels, except that for the last stage, and the temperature dynamics in the distillate tray are not included in the modeling. The dynamics for the salt concentration is also excluded because they have no direct effect on the other process states except through physical properties of the brine such as density and heat capacity. Our simulations revealed that the physical properties vary between +1 and -1 % over the plant temperature range due to changes in salt concentration. The mass holdup of the cooling brine inside the condenser tubes is assumed constant. The following mass and energy equations are written for each stage [2]:

Stage j (except the last stage)

- Mass balance of brine pool

$$\rho_{B,j} A_B \frac{dL_j}{dt} = B_{j-1} - B_j - V_j \quad (2.71)$$

- Energy balance of brine pool

$$\rho_{B,j} A_B L_j C_{p_{B,j}} \frac{dT_{Bj}}{dt} = B_{j-1} C_{p_{B,j}} (T_{B,j-1} - T_{B,j}) - V_j (\lambda_{c,j} - C_{p_{B,j}} (T_{B,j} - T_o)) \quad (2.72)$$

- Mass balance in distillate tray

$$D_j = D_{j-1} + V_j \quad (2.73)$$

- Energy balance of condenser tubes

$$M_{C,j}Cp_{C,j} \frac{dT_{C,j}}{dt} = B_0Cp_{C,j}(T_{C,j+1} - T_{C,j}) + U_j A_{HC} \Delta T_j \quad (2.74)$$

$$U_j A_{HC} \Delta T_j = V_j \lambda_j \quad (2.75)$$

(for the rejection section the see water feed W_F is used instead of B_0 in (2.74))

Last stage, N

- Mass balance in brine pool

$$\rho_{B,j} A_B \frac{dL_N}{dt} = B_{N-1} - B_N - V_N + W_{mk} - B_0 \quad (2.76)$$

- Energy balance in brine pool

$$\rho_{B,j} A_B L_N Cp_{B,j} \frac{dT_{B,N}}{dt} = B_{N-1} Cp_{B,j} (T_{B,N-1} - T_{B,N}) - V_N (\lambda_N - Cp_{B,j} (T_{B,N} - T_o)) + W_{mk} Cp_{B,j} (T_{C,3} - T_{B,N}) \quad (2.77)$$

- Mass balance in distillate tray

$$D_N = D_{N-1} + V_N \quad (2.78)$$

- Energy balance of condenser tubes

$$M_{C,N} Cp_{C,N} \frac{dT_{C,N}}{dt} = W_F Cp_{C,N} (T_F - T_{C,N}) + U_N A_{HR} \Delta T_N \quad (2.79)$$

$$U_N A_{HR} \Delta T_N = V_N \lambda_N \quad (2.80)$$

Splitter

$$W_F = Rej + W_{mk} \quad (2.81)$$

Brine Heater

- Energy Balance equation

$$M_{BH} Cp_{B,j} \frac{dT_{B0}}{dt} = B_0 (Cp_{C,1} T_{C,1} - Cp_{B0} T_{B0}) + W_s \lambda_s \quad (2.82)$$

Additional relations:

In the above model equations the brine flow and the brine level in each stage are correlated as follows:

$$B_j = wL_j K_j \sqrt{\rho_{B,j}(P_{j-1} - P_j + \rho_{B,j}g(L_j - Ch_j))} \quad (2.83)$$

Similarly, the distillate flow is correlated to the distillate level as follows:

$$D_j = C_{D,j} \sqrt{\rho_{D,j}gL_{D,j}} \quad (2.84)$$

The temperature difference used in the above energy balances is defined as follows:

$$\Delta T_i = T_{B,i} - 0.5(T_{C,i} + T_{C,i+1}) \quad (2.85)$$

Note that λ_j is computed at T_{Bj} while $\lambda_{c,j}$ is computed at the distillate temperature, which is assumed to be equal T_{Bj} minus the boiling point rise at the j^{th} stage (BPR_j). In the original model [2-4], the physical properties for each stage in the above model, i.e. $\rho, Cp, \lambda, U, M_c, M_{BH}, BPR$ and the vapor pressure (P) are estimated through empirical correlation.. Industrial values were used for the plant design parameters such as $C, h, A_B, A_{HC}, A_{HR}$ and w . Moreover, realistic values for the size and number of tubes were used in computing U, M_c and M_{BH} . The definition of all parameters of the model equations is given in the next table.

2.6.3 Process parameters and variables

<i>Variable</i>	<i>Description</i>	<i>Value</i>	<i>Units</i>
A_B	Cross sectional area for the brine chamber,	1260	m ²
A_{HR}	Heat transfer area for condenser tube at the rejection sections	7919.1	m ²
A_{HC}	Heat transfer area for condenser tube at the recover sections	77314.8	m ²
B	Inter stage Brine flow rate	Calc	ton/min
B_0	Recycle brine flow rates	217.257	ton/min
B_D	blow-down flow rates	29.3	ton/min
C	Orifice contraction coefficient	0.625	
C_D	Discharge coefficient for the distillate tray	1.0	
C_{pC}	Heat capacity for the brine in the condenser tube	Calc.	kJ/kg °C
C_{pB}	Heat capacity for the brine in the flash chamber,	Calc.	kJ/kg °C

D	Distillate flow rate	Calc.	ton/min
g	Gravitational constant	9.8	
h	Orifice height	0.11	m
K	Orifice discharge coefficient	0.68	
L	Brine level	Calc.	m
L_D	distillate level	Calc.	m
M_C	Liquid holdup for the condenser tube	23654.0	Kg
M_{BH}	Liquid holdup for the brine heater	34736.09	Kg
N	Total number of stages	22	
P	<i>Vapor pressure</i>	Calc.	Bar
Rej	Reject flow rate,	95.35	ton/min
T_o	Reference temperature	0	°C
T_F	Sea Water feed temperature	35	°C
T_B	Brine temperature	Calc.	°C
T_C	condenser temperature	Calc.	°C
T_s	Steam temperature	98.1	°C
T_{B0}	Top brine temperature,	93	°C
U	Overall heat transfer coefficient for the condenser tube	35	kJ/min °C m ²
U_s	Overall heat transfer coefficient for the brine heater	49.5	kJ/min °C m ²
V	Vapor rate, ton/min	Calc.	ton/min
X	Salt concentration	Calc/	kg/kg
W_D	distillate product flow rate	19.2	ton/min
W_F	Seawater feed flow rate respectively,	143.816	ton/min
W_S	Steam flow rate	2.452	ton/min
W_{mk}	Make up flow rate,	48.466	ton/min
w	Orifice width	0.5	m
w_N	Orifice width for stage N	3	m
ρ_B	Density of brine	Calc/	kg/m ³
ρ_D	Density of Distillate	1000	kg/m ³
λ	Latent heat for vaporization,	Calc.	kJ/kg
λ_c	Latent heat for vaporization at the distillate temperature	Calc.	kJ/kg
λ_s	Latent heat for steam,	Calc.	kJ/kg

2.7 TWO CSTRs IN SERIES

2.7.1 Process Description and Flow Sheet

Consider two CSTRs in series with an intermediate mixer as shown in Fig. 2.6. A chemical exothermic reaction of the form of: $A \rightarrow B$ takes place in the liquid phase. The reaction rate is considered to be first order in the reactant species. The feed to the first reactor is a pure species A with volumetric flow rate Q_{11} at ambient temperature. The liquid inside the reactor converts partially to species B . The heat released from the chemical reaction is removed by cooling water with volumetric flow rate Q_{cw1} and temperature T_{cw1} . The outlet of the first reactor has a volumetric flow rate Q_1 and temperature T_1 , and it is mixed with a fresh feed of pure component A . The product of the mixer is then fed to another reactor where the same first order reaction takes place. Water at ambient temperature is also used to cool the second reactor. The outlet flow rates are considered to be driven by the hydrostatic pressure in each tank, thus it related to the square root of the liquid holdup inside the reactor.

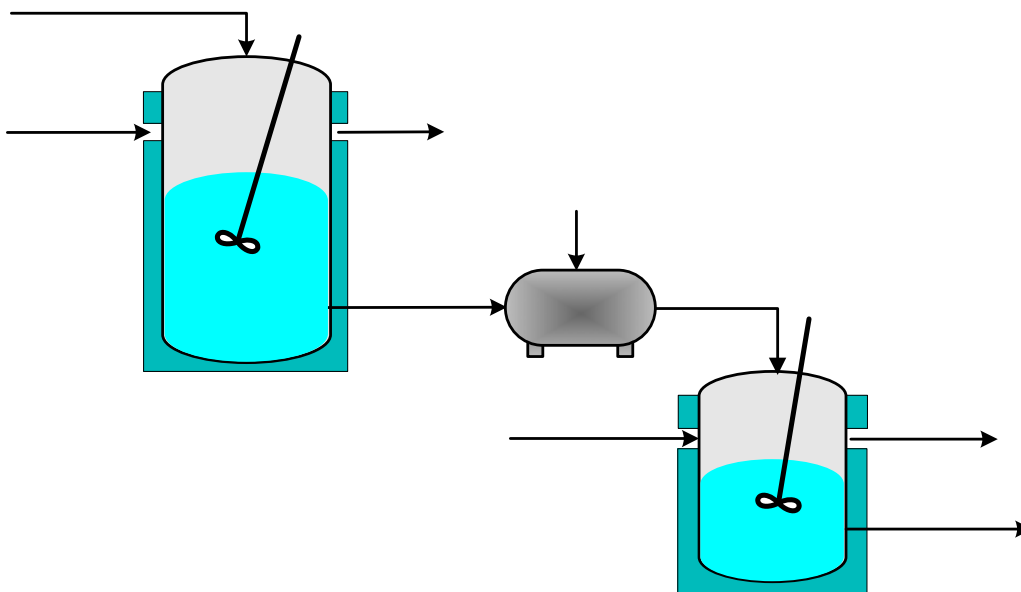


Fig. 2.6 Flow Sheet for two CSTRs in series

2.7.2 The Process Model

The following modeling equations are taken from [7]. State variables are used to describe the process variables. The definition of the states is given in section 2.7.3.

$$Q_{11}, C_{A1}, T_{11}$$

$$\dot{x}_1 = Q_{11} - K_{v1}\sqrt{x_1} \quad (2.86)$$

$$x_1\dot{x}_2 = Q_{11}(C_{11} - x_2) - K_1x_1x_2 \quad (2.87)$$

$$x_1\dot{x}_3 = K_1x_1x_2\Delta H + Q_{11}(T_{11} - x_3) - UA_1(x_3 - x_4) \quad (2.88)$$

$$V_{j1}\dot{x}_4 = Q_{cw1}(T_{cw1} - x_4) + UA_1(x_3 - x_4) \quad (2.89)$$

$$\dot{x}_5 = Q_{12} + K_{v1}\sqrt{x_1} - K_{v2}\sqrt{x_5} \quad (2.90)$$

$$x_5\dot{x}_6 = Q_{12}(C_{12} - x_6) - K_2x_5x_6 + K_{v1}\sqrt{x_1}(x_2 - x_6) \quad (2.91)$$

$$x_1\dot{x}_7 = K_2x_5x_6\Delta H + Q_{12}(T_{12} - x_7) + K_{v1}\sqrt{x_1}(x_3 - x_7) - UA_2(x_7 - x_8) \quad (2.92)$$

$$V_{j2}\dot{x}_8 = Q_{cw2}(T_{cw2} - x_8) + UA_2(x_7 - x_8) \quad (2.93)$$

Additional relations:

$$K_1 = k_0 \exp(-E/RT_1) \quad (2.94)$$

$$K_2 = k_0 \exp(-E/RT_2) \quad (2.95)$$

2.7.3 Process parameters and variables

<i>Variable</i>	<i>Description</i>	<i>Value</i>	<i>Units</i>
C_{11}	Feed concentration for component A	20	mole/m ³
C_{12}	Feed concentration for component A	20	mole/m ³
E/R	Activation energy	600	K
K_{v1}	Orifice constant for valve 1	0.16	m ^{3/2} /s
K_{v2}	Orifice constant for valve 2	0.256	m ^{3/2} /s
k_0	Pre-exponential factor	2.7×10^8	1/s
k_1	Reaction rate in CSTR 1		1/s
k_2	Reaction rate in CSTR 2		1/s
Q_{11}	Feed rate for CSTR 1	0.339	m ³ /s
Q_{12}	Feed rate for mixer	0.261	m ³ /s
Q_{cw1}	Cooling water feed rate to CSTR 1	0.45	m ³ /s
Q_{cw1}	Cooling water feed rate to CSTR 1	0.272	m ³ /s
T_{11}	Feed temperature to CSTR 1	300.0	K

T_{12}	Feed temperature to CSTR 2	300.0	K
T_{cw1}	Cooling water temperature to CSTR 1	300.0	K
T_{cw2}	Cooling water temperature to CSTR 2	300.0	K
UA_1	Heat transfer coefficient times the heat transfer area for CSTR 1	0.35	m ³ /s
UA_2	Heat transfer coefficient times the heat transfer area for CSTR 2	0.35	m ³ /s
V_{j1}	Cooling jacket volume for CSTR 1	1.0	m ³
V_{j1}	Cooling jacket volume for CSTR 2	1.0	m ³
x_1	Liquid holdup in CSTR 1	4.4891016	m
x_2	concentration of component A in CSTR1	0.0840220	mole/m ³
x_3	Temperature in CSTR1	362.99526	K
x_4	Temperature of coolant in CSTR1	327.56042	K
x_5	Liquid holdup in CSTR 2	5.4931641	m
x_6	concentration of component A in CSTR2	0.0503550	mole/m ³
x_7	Temperature in CSTR2	362.99495	K
x_8	Temperature of coolant in CSTR2	335.44732	K
ΔH	Heat of reaction	5	m ³ K/mole

2.8 FLUID CATALYTIC CRACKING UNIT

2.8.1 Process Description and Flow Sheet

Fluid Catalytic Cracking (FCC) is one of the most important units in the petroleum refining industry for the conversion of heavy gas oil to gasoline and light hydrocarbons. The performance of the FCC units plays major role on the overall economics of petroleum refineries. FCCU receives a number of hydrocarbon feed-streams with different molecular weight distribution from several refinery units and cracks the heavier components in these streams to more valuable lighter ones.

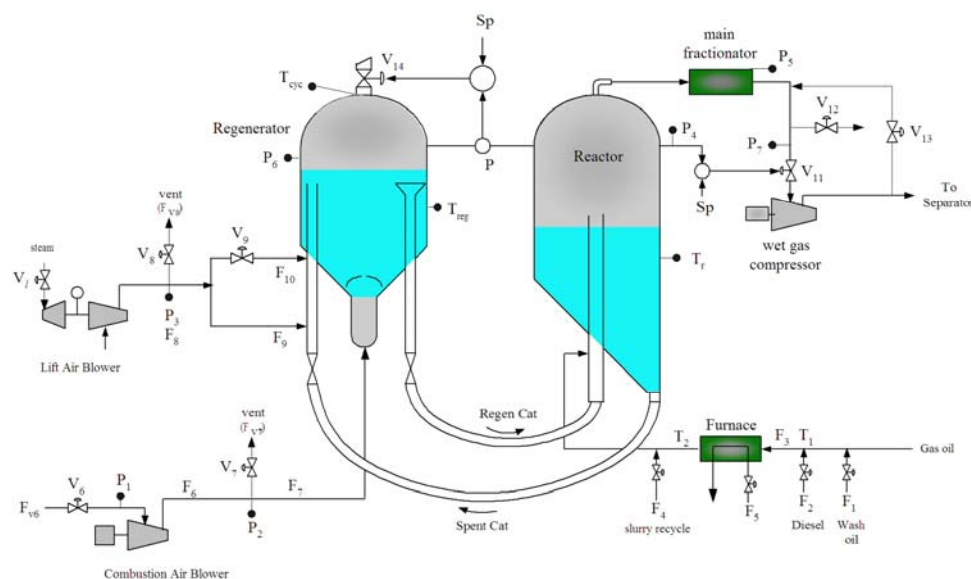


Fig. 2.7 Flow sheet for FCCU process

The FCCU as Shown in Fig. 2.7 consists of two major processes; a reactor and a regenerator. In the reactor, cracking reaction occurs and coke is deposited on the catalyst. The reaction product is passed to the main fractionator for heat recovery and separation into various product streams. The spent catalyst is sent to the regenerator section where the coke is burnt by excess of oxygen to form carbon monoxide and carbon dioxide. The gaseous products of the combustion reaction leave the regenerator section through the cyclones as stack gas. The regenerated catalyst is recycled to the reactor.

The catalyst is transferred back and forth between the reactor and regenerator through the catalyst U-bend. Air is injected at the bottom of the regenerator lift pipe to

assist the circulation of the catalyst. Further detailed description of the process can be found in [13].

2.8.2 The Process Model

The process dynamic equation can be found in the previous reference [13]. The model equations are lengthy that we believe not to include them.

2.8.3 Process Parameters and Variables*

<i>Variable</i>	<i>Description</i>	<i>Value</i>	<i>Units</i>	<i>Type</i>
C_{co}	Concentration of carbon monoxide in stack gas	37	ppm	State/output
C_{O_2}	Concentration of Oxygen in stack gas	0	ppm	State/output
C_{rge}	Weight fraction of coke on regenerated catalyst	0.0008475	ICFM	State/output
C_{sc}	Weight fraction of coke on spent catalyst	0.0078	ICFM	State/output
F_{sukka}	Combustion air blower inlet suction flow	49465	ICFM	algebraic
F_{sucla}	Lift air blower inlet suction flow	11750	ICFM	algebraic
F_{sucwg}	Wet gas compressor suction flow	19011	ICFM	algebraic
F_{surca}	Combustion air blower inlet surge flow	45100	ICFM	constant
F_{surla}	Lift air blower inlet surge flow	9571.6	ICFM	algebraic
F_{surwg}	Wet gas compressor surge flow	11700	ICFM	constant
F_{air}	Air flow rate into regenerator	75.5375	lb/s	algebraic
F_1	Flow of wash oil to reactor riser	13.8	lb/s	input
F_2	Flow of diesel to reactor riser	0.0	lb/s	input
F_3	Fresh feed flow rate to reactor riser	126	lb/s	input
F_4	Slurry flow rate to reactor riser	5.25	lb/s	input
F_5	Fuel flow rate to furnace	34	lb/s	input
F_6	Combustion air blower throughput,	60.9656	lb/s	algebraic
F_7	Combustion air flow to regenerator	60.9656	lb/s	Algebraic
F_8	lift air blower throughput	14.5719	lb/s	algebraic
F_9	Combustion air flow to regenerator	14.5719	lb/s	algebraic
F_{10}	spill air flow to regenerator	0.0	lb/s	algebraic
F_{11}	Wet gas flow to the vapor recovery	1.1275	mole/s	Algebraic

	unit			
F_{v6}	Flow through combustion air blower suction valve,	60.1634	lb/s	Algebraic
F_{v7}	Flow through combustion air blower vent valve,	0	lb/s	Algebraic
F_{v8}	Flow through lift air blower vent valve,	0	lb/s	Algebraic
F_{v11}	Flow through wet gas compressor suction valve	1.1275	lb/s	algebraic
F_{v12}	Flow through wet gas compressor vent valve	0	lb/s	Algebraic
F_{v13}	Flow through wet gas compressor anti-surge valve	0	lb/s	Algebraic
Lsp	Level of catalyst in standpipe	10.1596	ft	Algebraic
n	Amount of gas	246.25	mole	state
P_{blp}	Pressure at bottom of lift pipe	32.1	Psia	Algebraic
P_1	Combustion air blower suction pressure	14.6421	Psia	State
P_2	Combustion air blower surge pressure	35.2159	Psia	State
P_3	Lift air blower discharge pressure	40.5944	Psia	state
P_4	Reactor Pressure	32.8244	Psia	algebraic
P_5	Reactor fractionation pressure	23.3244	Psia	State
P_6	Regenerator Pressure	29.6707	Psia	State
P_7	Wet gas compressor suction pressure	22.4988	psia	State
T_{cyc}	Regenerator cyclone temperature	1279.2	°F	State
T_r	Reactor temperature	992.6582	°F	State
T_{reg}	Regenerator bed temperature	1286.4	°F	State
T_1	Fresh feed temperature to furnace	460.9	°F	Input
T_2	Fresh feed temperature to reactor	667.2611	°F	state
T_3	Furnace firebox temperature	1607.6	°F	State
V_6	Combustion air blower suction valve position	1		Input
V_7	Combustion air blower vent valve position	0		Input
V_8	Lift air blower vent valve position	0		Input
V_9	Spill air valve position	0		Input
V_l	List air steam valve	0.4313		Input
V_{11}	Wet gas compressor suction valve position	0.95		Input
V_{12}	Wet gas flare valve position	0		Input

V_{13}	Wet gas compressor vent valve position	0	Input
V_{14}	Stack gas valve position	0.612	Input
W_r	Inventory of catalyst in reactor	101696.89 lb	state
W_{reg}	Inventory of catalyst in regenerator	273763.07 lb	State
W_{sp}	Inventory of catalyst in regenerator spent pipe	3200.27 lb	State
ρ_{lift}	Density of catalyst in lift pipe	3.2 lb/ft ³	State

* definition and numerical values of various process parameters are given in the cited reference.

The system has three major PI control loops which are set as:

Control loop	k_c	τ_I
$P_4 \rightarrow V_{11}$	0.1	0.04
$\Delta P \rightarrow V_{14}$	0.08	0.03
$F_{air} \rightarrow V_l$	0.01	0.0025

The process has several equipment and operational constraints as follows:

Flows:

$$\begin{aligned}
 0 &\leq F_1 \leq 17 \\
 0 &\leq F_2 \leq 16 \\
 0 &\leq F_3 \leq 144 \\
 0 &\leq F_4 \leq 10 \\
 0 &\leq F_5 \leq 20
 \end{aligned}$$

Valves:

$$0 \leq V_i \leq 1; \quad i = 1, 14$$

Vessels:

$$\begin{aligned}
 P_6 &< 39.7 \text{ psig} \\
 P_5 &< 39.7 \text{ psig}
 \end{aligned}$$

Compressor surge limit (level: 10)

Lift air:	$F_{suc} - F_{sur} > 0$
Combustion air	$F_{suc} - F_{surg} > 0$
Wet gas	$F_{suc} - F_{sur} < 0$

Total combustion in regenerator (level: 9.5)

$$C_{O,sg} > 1.5\%$$

$$T_{\text{reg}} > 1265 \text{ }^{\circ}\text{F}$$

Or

$$T_{\text{cyc}} - T_{\text{reg}} < 20 \text{ }^{\circ}\text{F}$$

$$T_{\text{cyc}} < 1310 \text{ }^{\circ}\text{F}$$

$$C_{\text{CO,sg}} < 350 \text{ ppm}$$

Differential pressure: (level 8)

$$-5.0 \leq \Delta P \leq -2.0 \text{ psi}$$

Standpipe level: (level lower limit = 10, upper limit = 8)

$$0 \leq L_{\text{sp}} \leq 20 \text{ ft}$$

Riser Temperature: (level 10)

$$T_{\text{r}} \leq 995 \text{ }^{\circ}\text{F}$$

Furnace Temperature: (level 9)

$$T_3 \leq 1700 \text{ }^{\circ}\text{F}$$