Advanced Reaction Engineering

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12/11/12

Illustrative Example

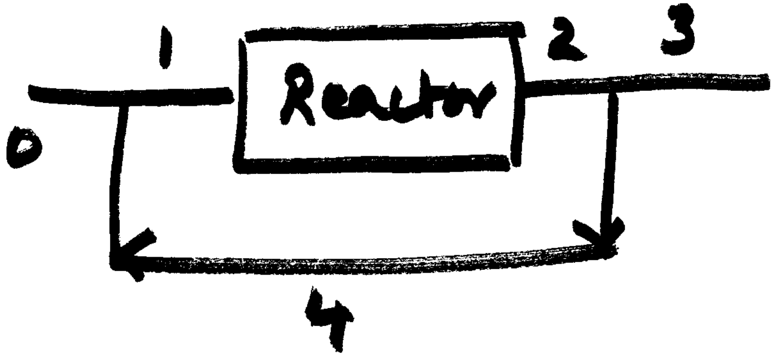
Recycle Effects in Process

2 NOV 12
1030–1130

Recycle Reactors

Design Equation.

$$\frac{V}{F_{A0}} = (R+1)\int_{X_1}^{X_3} \frac{dx}{-r_A}.$$



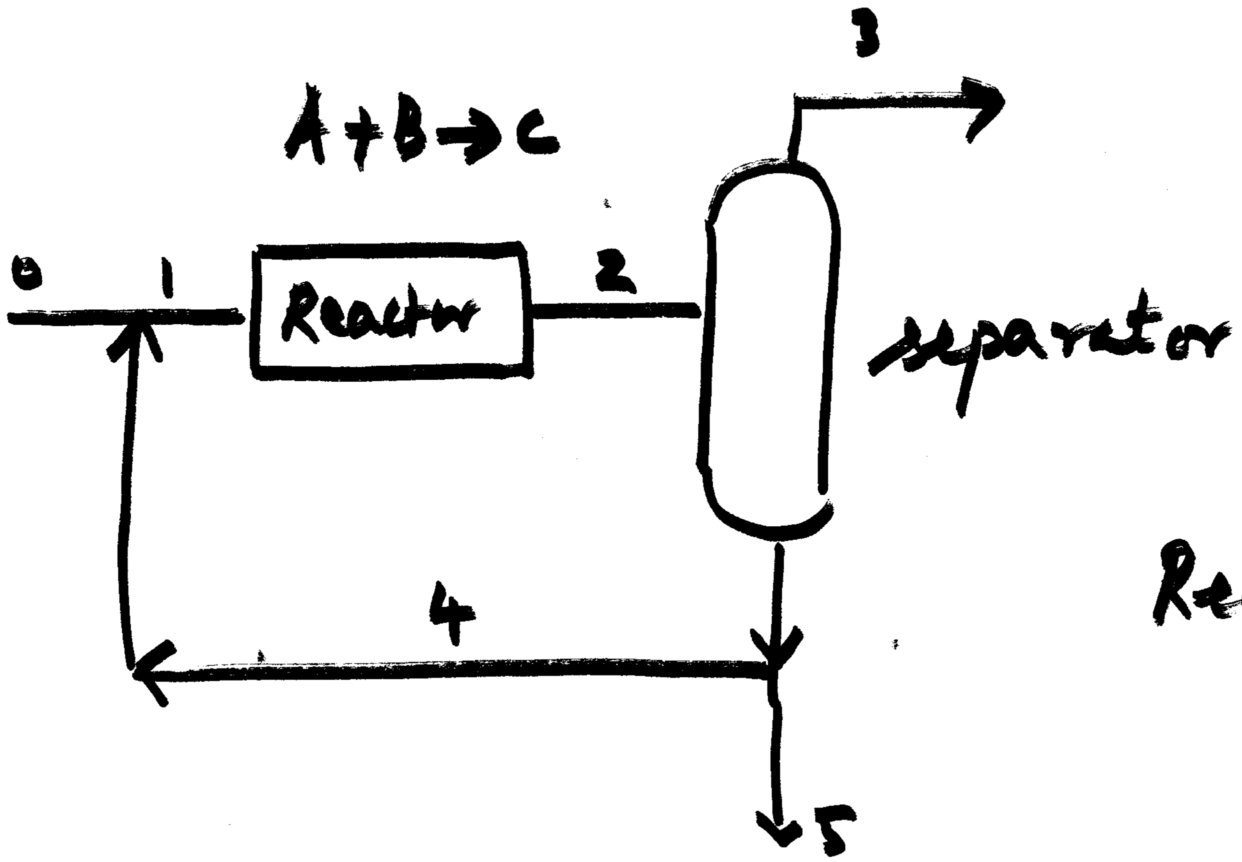
$R = 0$ PFR

$R \to \infty$ CSTR

$R\ (0 + \infty)$

$X_2 = X_3$

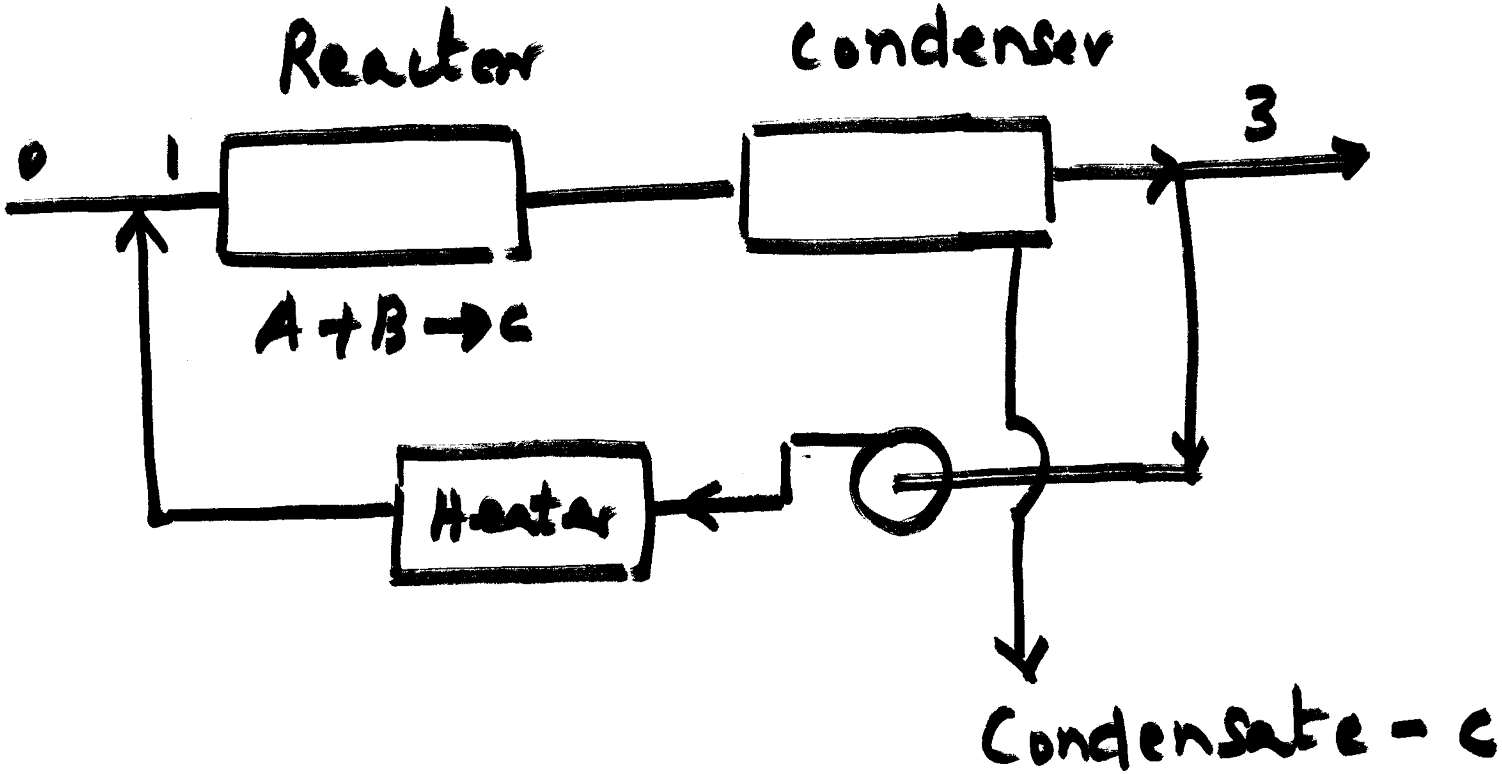
$$X_1 = \frac{R}{R+1} X_3 = \frac{R}{R+1} X_2$$

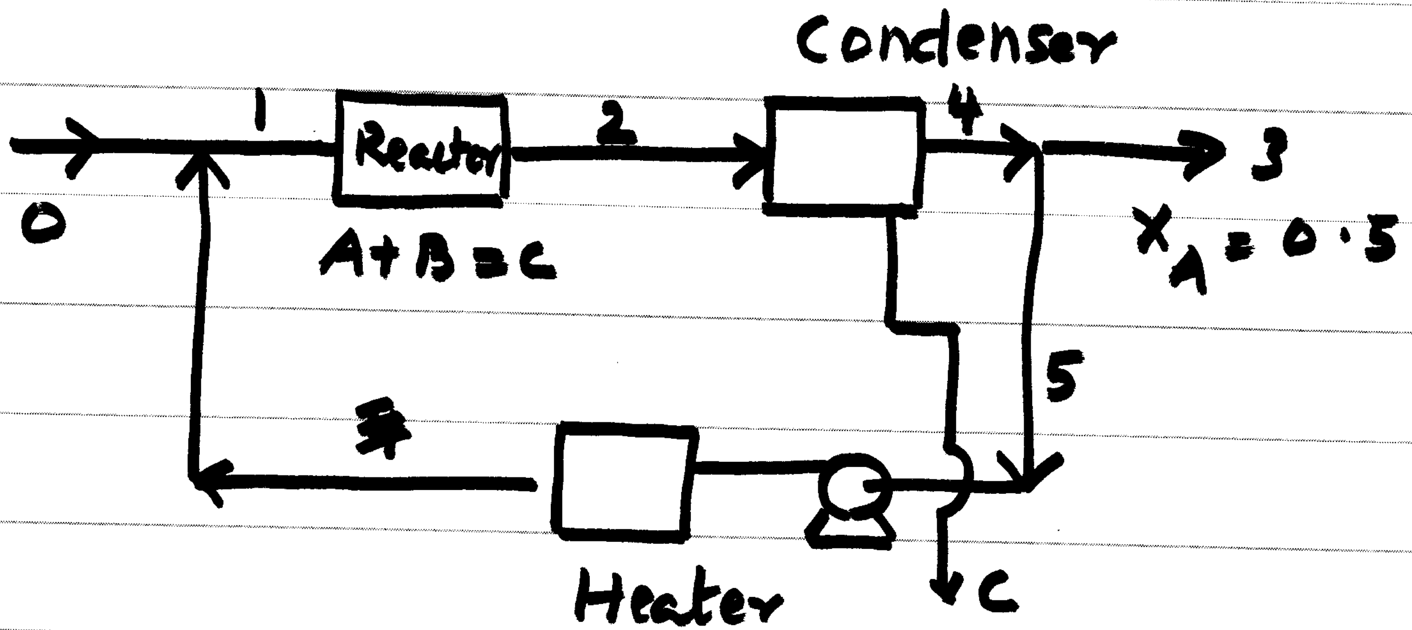


Reactor

CSTR

PFR.


Reactor
Condenser
0
1
3
A + B → C
Heater
Condensate - C



$F_{A0} = F_{B0} = 1$ kmol/hr

T: 570 C

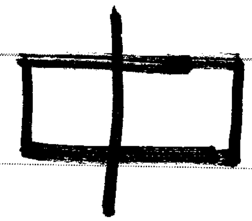
P: 1atm

Vap C = 0.2 atm at 45C.

Recycle Ratio R=4

x_A = Desired = 0.5

Flow at any position in Reactor



A $(R+1)F_{A0}(1-x_A)$

B $(R+1)F_{A0}(1-x_A)$

C $(R+1)F_{A0}\,x_A$

$$F_t = 2(R+1)F_{A0}(1-x_A) + (R+1)F_{A0}\,x_A$$

At incipient condensation

$P = 1\,\text{atm}$

$P_c^* = 0.2$

$$0.2 = \frac{(R+1)F_{A0}X_s}{2(R+1)F_{A0}(1-X_s) + (R+1)F_{A0}X_s}$$

$$0.2 = \frac{X_s}{2(1-X_s)+X_s} = \frac{X_s}{2-X_s}$$

$$X_s = 0.4/1.2 = 0.33$$

upto $X_A = X_s = 0.33$ no liquid is found in stream 6 since all such C will be in gas phase

Stoichiometric Table

A	$(R+1)\, F_{A0}\, (1-x)$	(g)
B	$(R+1)\, F_{A0}\, (1-x)$	(g)
C	$(R+1)\, F_{A0}\, x$	(g)

$$\underline{\overline{F_t = (R+1)\, F_{A0}\, (2-x)}} \quad \text{for} \quad x < x_s$$

Stoichiometric Table $X > X_s$

A	$(R+1)\,F_{A0}\,(1-X)$	(g)
B	$(R+1)\,F_{A0}\,(1-X)$	(g)
C	$(R+1)\,F_{A0}\,X_s$	(g)

$$F_t = (R+1)\,F_{A0}\,(2-2X+X_s) \qquad X > X_s$$

$$\frac{v}{v_0} = \frac{F_t}{F_{t0}} = \frac{(2-2X+X_3)(R+1)F_{A0}}{2}$$

$\because$ T, P, Z constant

Note position '0' is outside recycle loop

Material Balance for A at '1'

$$F_{A1} = (R+1)F_{A0}(1-X_1) = RF_{A0}(1-X_3) + F_{A0}$$

$$(R+1)(1-X_1) = R(1-X_3)+1$$

gives

$$X_1 = \frac{RX_3}{(R+1)}$$

Note $X_3 = X_2$ by definition

$$C_A = \frac{F_A}{v} = \frac{2(R+1)F_{A0}(1-x)}{v_0(2-2x+x_s)} \qquad \underline{x > x_s}$$

Note '0' refers to position outside recycle loop

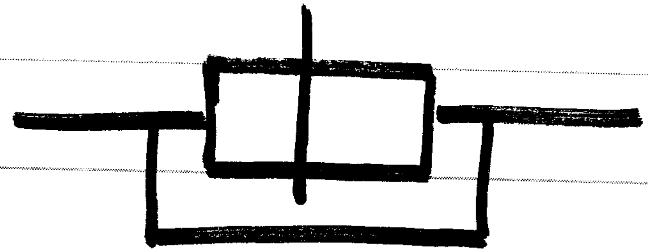
$$C_A = \frac{F_A}{v} = \frac{2(R+1)F_{A0}(1-x)}{v_0(2-\cancel{2}x)} \qquad x < x_s$$

So

$$C_A = \frac{2(R+1)C_{A0}(1-x)}{(2-\cancel{2}x)} \qquad x < x_s$$

$$= \frac{2(R+1)C_{A0}(1-x)}{(2-2x+x_s)} \qquad x > x_s$$

$$\frac{dF}{dV} = r_A = -kC_A^2$$



$A + B \rightarrow C$

$$-(R+1)F_{A0}\frac{dx}{dV} = -kC_A^2$$

$$= kC_{A0}^2\left[\frac{2(R+1)(1-x)}{2-x}\right]^2$$

for 0 to x_s

$$\frac{dx}{d\tau} = kC_{A0}\left[\frac{2(1-x)}{2-x}\right]^2(R+1)$$

for 0 to x_s

$$\tau = V/v_0$$

$$\frac{dF_A}{dV} = r_A = -kC_A$$

$$-(R+1)F_{A0}\frac{dX}{dV} = -kC_A^2$$

$$(R+1)F_{A0}\frac{dX}{d\tau} = kC_{A0}^2\left[\frac{2(R+1)(1-X)}{2-2X+X_S}\right]^2$$ for X_S upto X

$$\frac{dX}{d\tau} = kC_{A0}\left[\frac{2(1-X)}{2-2X+X_S}\right]^2(R+1)$$

$$v_0 = \frac{F_{t_0} RT}{P} = \frac{2(0.082)843}{1.0}$$

$$= 138 \ m^3/hr.$$

$$C_{A0} = \frac{P(0.5)}{RT} = \frac{(1)(0.5)}{(0.082)843} = (3.6)10^{-3} \frac{gmol.}{L}$$

$$C_{A0} k = (3.6) 10^{-2} /s$$

$$k = 10/s$$

Value of Integral $= \tau = 1.0$ Second.

$V_R = (\tau) v_0 = 38$ Lit

$$\tau = \int_{X_s}^{X} \frac{(2 - 2X + X_s)^2}{kC_{A0}[R+1]\,4(1-X)^2}\,dX$$

$$+ \int_{0}^{X_s} \frac{(2 - X)^2}{kC_{A0}(R+1)\,4(1-X)^2}$$

Putting numbers and integratng numerically

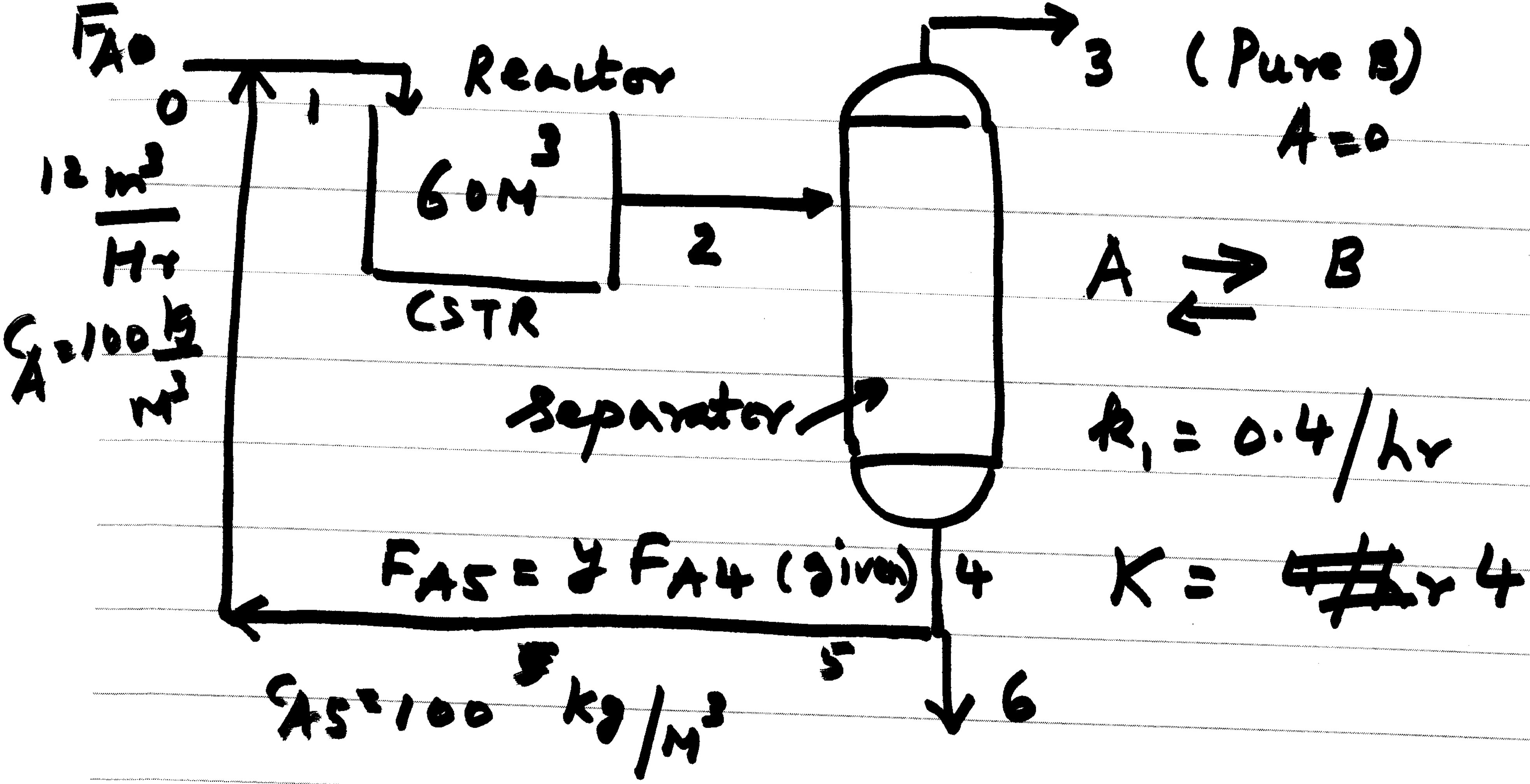
$$SO_2 + \frac{1}{2} O_2 = SO_3$$

SO_3 is a condensible gas. Such condensation effects to be accounted.

38 lit can process $(64) \frac{kg}{hr}$ SO_2 with $X_A = 0.5$

So $76\,m^3$ of catalyst can process..

$$\frac{(32)}{38}(76)\,10^3\ kg/hr = 64 \frac{ton}{hr}$$



Product B is worth Rs 2/kg

Operating Cost Rs 50/M^3 entering Separator

Find y which maximises profit

Material Balance

$$F_{A1} = F_{A0} + F_{A5} \quad \text{-- (1)}$$

$$F_{A2} = F_{A1}(1-\alpha)$$

where α is conversion defined with respect to position 1

$$F_{A3} = 0 \quad \text{(given)}$$

$$F_{A4} = F_{A1}(1-\alpha) \quad \text{-- (2)}$$

$$F_{A5} = y\, F_{A4} \quad \text{(opt } y \text{ to be found) -- (3)}$$

$$F_{A1} = F_{A1} + F_{A5}$$

$$F_{A1} = F_{A0} + y F_{A4}$$

$$= F_{A0} + y F_{A1}(1-\alpha)$$

$$\boxed{F_{A1} = \frac{F_{A0}}{1 - y(1-\alpha)}}$$

Now $C_{A1} = C_{A0}$ (given)

$$v_1 = F_{A1}/C_{A1} = \frac{F_{A0}}{[1-y(1-\alpha)]\, C_{A0}} = \frac{v_0}{1-y(1-\alpha)}$$

$$C_{A1} = C_{A0}$$

$$v_1 = \frac{F_{A1}}{C_{A1}} = \frac{F_{A0}}{(1-y(1-\alpha))C_{A0}} = \frac{v_0}{1-y(1-\alpha)}$$

$$C_{B2} = \frac{F_{B2}}{v_2} = \frac{F_{A1}\alpha}{v_1} \qquad (\because v_2 = v_1)$$

$$= C_{A1}\alpha = C_{A0}\alpha$$

$$C_{A2} = \frac{F_{A2}}{v_2} = \frac{F_{A1}(1-\alpha)}{v_1} = C_{A1}(1-\alpha)$$

$$= C_{A0}(1-\alpha)$$

CSTR Equation

$$A \underset{2}{\overset{1}{\rightleftharpoons}} B$$

$$V = \frac{F_{A1}\,\alpha}{(-r_A)_2} = \frac{F_{A0}\,\alpha}{[1-y(1-\alpha)][k_1 C_{A2} - k_2 C_{B2}]}$$

$$\boxed{r_A = k_2 C_{B2} - k_1 C_{A2}}$$

$$V = \frac{F_{A0}\,\alpha}{[1-y(1-\alpha)][k_1 C_{A0}(1-\alpha) - k_2 C_{A0}\alpha)]}$$

$$V = \frac{v_0\,\alpha}{[1-y(1-\alpha)][k_1(1-\alpha) - k_2\alpha]}$$

$$\tau = \frac{\alpha}{(1-y(1-\alpha))(k_1(1-\alpha) - k_2\alpha)} \quad \text{—} \quad (4)$$

Profit Function

$$P = F_{B2}\,\beta_B - v_2\,\beta_0$$

$$v_2 = v_1$$

β_B : Rs 2/kg β_0 : Rs 50/m^3 $v_1 = \dfrac{v_0}{1-y(1-\alpha)}$.

$$P = (F_{A1}\alpha)\,2 - \frac{50\,v_0}{1-y(1-\alpha)}$$

$$\boxed{P = \frac{2F_{A0}\alpha}{1-y(1-\alpha)} - \frac{50\,v_0}{1-y(1-\alpha)} \quad \text{--- (5)}}$$

From (4)

$$1 - y(1-\alpha) = \frac{\alpha}{\left[k_1(1-\alpha) - k_2\alpha\right]\tau} \quad - (6)$$

substituting for $1 - y(1-\alpha)$ from (6) in (5)

$$P = \frac{\left[2 F_{A0}\alpha - 50 v_0\right]\tau\left\{k_1(1-\alpha) - k_2\alpha\right\}}{\alpha}$$

$$P = \tau\left\{k_1(1-\alpha) - k_2\alpha\right\}\left[2 F_{A0} - \frac{50 v_0}{\alpha}\right] \quad - (7)$$

Data

$\tau = 60/12 = 5$ hrs

$k_1 = 0.4/\text{hr}$; $k_2 = 0.1/\text{hr}$

$F_{A0} = 1200$ kg/hr

$C_{A0} = 100$ kg/m^3

$v_0 = 12$ m^3/hr

Putting numbers in (7)

$$P = 5\{0.4(1-\alpha) - 0.1\alpha\}\left\{2400 - \frac{600}{\alpha}\right\}$$

$$= (2 - 2.5\alpha)\left(2400 - \frac{600}{\alpha}\right) \quad \ldots (8)$$

From (6)

$$y = \left[1 - \frac{\alpha}{\tau\left[k_1(1-\alpha) - k_2\alpha\right]}\right] \Big/ (1-\alpha).$$

α - is conversion w.r.t to F_{A1}. α cannot be 1 since we have a reversable reaction.

α	y
0	1
0.4	finite
0.8	finite

$\frac{d\alpha}{dy}$ exists

$$P = (2 - 2.5\alpha)\left(2400 - \frac{600}{\alpha}\right)$$

$$\frac{dP}{d\alpha} = (2 - 2.5\alpha)\left(\frac{600}{\alpha^2}\right)$$

$$+ \left(2400 - \frac{600}{\alpha}\right)(-2.5)$$

$$\frac{dP}{dy} = \left(\frac{dP}{d\alpha}\right)\left(\frac{d\alpha}{dy}\right)$$

Since $\frac{d\alpha}{dy}$ exists we can set $\frac{dP}{d\alpha} = 0$

$$\frac{dP}{d\alpha} = 0$$

$$= \frac{1200}{\alpha^2} - \cancel{\frac{1500}{\alpha}} - 6000 + \cancel{\frac{1500}{\alpha}}$$

$$\frac{1200}{\alpha^2} = 6000$$

$$\alpha^2 = \left(1/5\right) \Rightarrow \alpha = \sqrt{0.2} = \underline{\underline{0.447}}$$

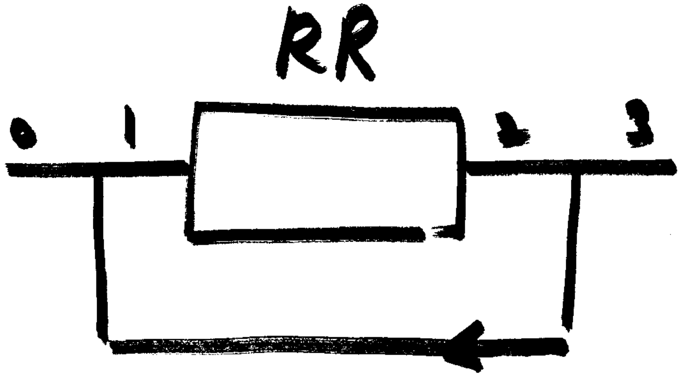
From (4)

$$\tau = \frac{\alpha}{(1 - y(1-\alpha))(k_1(1-\alpha) - k_2\alpha)}$$ we get

$$5 = \frac{0.447}{\{1 - y(1 - 0.447)\}\{0.4(1 - 0.447) - 0.1(0.447)\}}$$

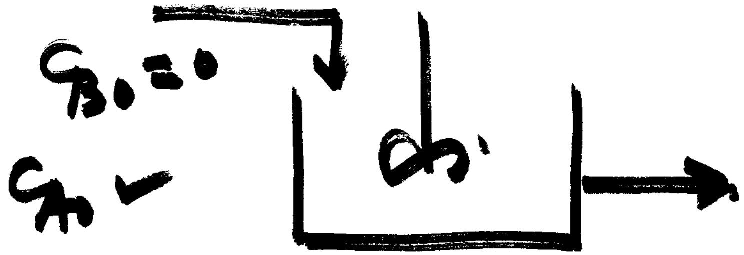
$$5 = \frac{0.447}{(1 - 0.553y)(0.1765)} \Rightarrow \underline{\underline{y = 0.89}}$$

Conversion $X = \frac{F_{B2}}{F_{A0}} = \frac{F_{A*}\alpha}{F_{A0}} = \frac{\alpha_1}{1-y(1-\alpha)} = \underline{\underline{0.88}}$



$A \rightarrow B$

$r_A = -k C_A C_B.$



$r_A = -k C_A C_B.$

ineffective for Autocat.