$$\alpha_{11} A_1 + \alpha_{12} A_2 + \dots \alpha_{1n} A_n = 0$$

$$\alpha_{21} A_1 + \alpha_{22} A_2 + \dots \alpha_{2n} A_n = 0$$

$$\alpha_{p1} A_1 + \alpha_{p2} A_2 + \dots \alpha_{pn} A_n = 0$$

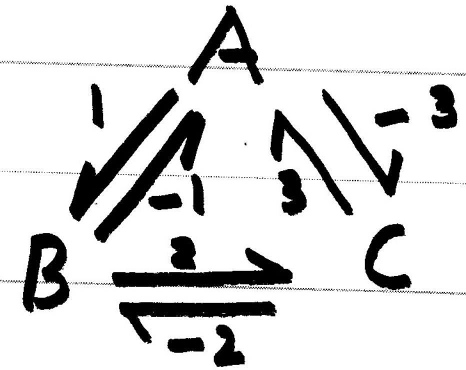
p – rxns.

n – Components

r – independent rxns.

$$\underline{A_{\cdot j} - A_{j_0}} = x_1 \alpha_{1j} + x_2 \alpha_{2j} + \cdots x_r \alpha_{rj}.$$

Q



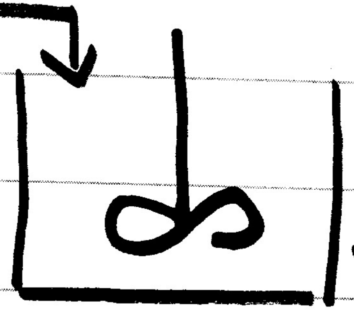
All Rxns instantaneous

T = 50 C

$K_1 = 1.0 = \frac{k_1}{k_{-1}}$

$K_2 = 2.0.$

F_{A0} 10 mol/s



$\rightarrow F_A$, F_B, F_C

$K_3 = 0.5$

Find Composition of system at steady state

All rxn are instantaneous

REACTION NETWORK

Forward

$B - A = 0$

$C - B = 0$

$A - C = 0$

$$\begin{bmatrix} -1 & 1 & 0 \\ 0 & -1 & 1 \\ 1 & 0 & -1 \end{bmatrix}$$

Reverse

$A - B = 0$

$B - C = 0$

$C - A = 0$

$$\begin{bmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \\ -1 & 0 & 1 \end{bmatrix}$$

Determinant zero; Rank $= 2$

$$
\begin{array}{c}
\begin{array}{ccc} A & B & C \end{array} \\
\begin{bmatrix}
-1 & 1 & 0 \\
1 & -1 & 0 \\
0 & -1 & 1 \\
0 & 1 & -1 \\
1 & 0 & -1 \\
-1 & 0 & 1
\end{bmatrix}
\end{array}
$$

Take any two independent set

$$A \rightarrow B \qquad x_1$$

$$B \rightarrow C \qquad x_2$$

$$F_A = F_{A0}(1 - x_1)$$

$$F_B = F_{A0}x_1 - F_{A0}x_2 + F_{B0}$$

$$F_C = F_{C0} + F_{A0}x_2$$

$$\frac{C_B}{C_A} = K_1 \qquad \frac{C_C}{C_B} = K_2$$

$$\frac{C_B}{C_A} = \frac{F_B}{F_A} = \frac{F_{A0}(X_1 - X_2)}{F_{A0}(1 - X_1)} = K_1 \quad - (1)$$

$$\frac{C_C}{C_B} = \frac{F_C}{F_B} = \frac{F_{A0}(X_2)}{F_{A0}(X_1 - X_2)} = K_2 \quad - (2)$$

From (2) $$X_2 = \frac{K_2 X_1}{(K_2 + 1)} \quad - (3)$$

From (1)

$$X_1 - X_2 = K_1 (1 - X_1)$$

$$X_1 \left\{ 1 + K_1 - \frac{K_2}{1+K_2} \right\} = K_1$$

$$X_1 = \frac{K_1}{1 + K_1 - K_2/(1+K_2)}$$

$F_A = 2.5$

$F_B = 2.5$

$F_C = 5.0.$

$$X_2 = \frac{K_2 X_1}{1+K_2}$$

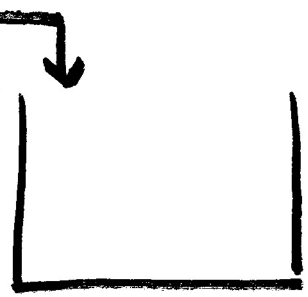
$K_1 = 1 \qquad K_2 = 2$

$$X_1 = \frac{1}{1+1 - 2/3} = 3/4 = 0.75;$$

$$X_2 = K_2 X_1/(1+K_2) = (2)(0.75)/(3) = 0.5$$

Q

$C = 10 \frac{mol}{s}$



$C \rightarrow A$ (1) X_1

$A \rightarrow B$ (2) X_2

$F_C = F_{C0}(1-X_1)$

$F_A = F_{A0} + F_{C0}(X_1 - X_2)$

$F_B = F_{B0} + F_{C0} X_2$

$$\frac{C_B}{C_A} = K_1$$

$$\frac{F_B}{F_A} = \frac{X_2}{X_1 - X_2} = K_1 \quad -(1)$$

$$\frac{C_C}{C_B} = K_2$$

$$\frac{1-X_1}{X_2} = K_2 \quad -(2)$$

$$X_2 = K_1 (X_1 - X_2)$$

$$X_2 (1 + K_1) = K_1 X_1$$

$$X_2 = \frac{K_1 \; X_1}{(1 + K_1)} \quad \ldots (3)$$

$$1 - X_1 = K_2 X_2$$

$$1 - X_1 = \frac{K_2 \; K_1 \; X_1}{1 + K_1}$$

$$X_1 \left[1 + \frac{K_1 K_2}{1 + K_1} \right] = 1$$

$$X_1 = \frac{1}{\left[1 + \frac{K_1 K_2}{(1 + K_1)} \right]}$$

$$K_1 = 1 ; \quad K_2 = 2$$

$$X_1 = \frac{1}{1 + 2/2} = 0.5$$

$$X_2 = \frac{(1)(0.5)}{2}$$

$$= 0.25$$

$$F_A = \cancel{F_{A0}} + F_{C0}\,(X_1 - X_2)$$

$$= 10\,(0.5 - 0.25) = 2.5\ \frac{m\Omega}{s}$$

$$F_B = \cancel{F_{B0}} + F_{C0}\,X_2$$

$$= (10)\,(0.25) = 2.5\ m\Omega/s$$

$$F_C = F_{C0}\,(1 - X_1) = 10\,(1 - 0.5) = 5\ \frac{m\Omega}{s}.$$

General Procedure

$$B \to C \qquad (1)$$
$$C \to A \qquad (2)$$

$$A_j - A_{j0} = X_1 \alpha_{1j} + X_2 \alpha_{2j}$$

$$F_A - \cancel{F_{A0}} = 0 + X_2$$

$$F_B - \cancel{F_{B0}} = -X_1 + 0$$

$$F_C - F_{C0} = X_1 - X_2$$

$$X_1 = \frac{-K_1 \cancel{K_2} F_{C0}}{1 + K_1 + K_1 K_2};$$

$$X_2 = F_{C0}/(1 + K_1 + K_1 K_2)$$

$$\frac{c_B}{c_A} = \frac{F_B}{F_A} = K_1$$

$$-\frac{X_1}{X_2} = K_1 \qquad (3)$$

$$\frac{c_C}{c_B} = \frac{F_{C0} + X_1 - X_2}{-X_1} = K_2 \qquad (4)$$

From (4)

$$F_{co} + X_1 - X_2 = -K_2 X_1 \qquad (5)$$

From (3)

$$X_1 = -\cancel{K_2 X_2} - K_1 X_2 \qquad - (6)$$

Substituting in (5)

$$F_{co} - K_1 X_2 - X_2 = -K_2(-K_1 X_2)$$

$$F_{co} = K_1 X_2 + X_2 + K_1 K_2 X_2$$

$$= X_2 (1 + K_1 + K_1 K_2)$$

$$X_2 = F_{co} / (1 + K_1 + K_1 K_2) \qquad - (7)$$

$$X_1 = -K_1 X_2$$

$$= \frac{-K_1 F_{C0}}{1 + K_1 + K_1 K_2} \quad - (8)$$

Putting numbers $K_1 = 1 \quad K_2 = 2, \quad F_{C0} = 10 \frac{ml}{s}$

$$X_2 = \frac{10}{1+1+2} = 2.5 \; ; \quad X_1 = -2.5$$

$$F_A = X_2 = 2.5 \text{ ml/s}$$

$$F_B = -X_1 = 2.5 \text{ ml/s}$$

$$F_C = 10 + X_1 - X_2 = 10 - 2.5 - 2.5 = 5 \frac{ml}{s}.$$

Instaintaneous & overall yields

$$A \rightarrow D$$
$$A \rightarrow U$$

Lets Take a PFR

$$\frac{dF_D}{dV} = r_D$$

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

$$\frac{dF_D}{dF_A} = \frac{r_D}{r_A} = -\phi$$ (is a +ve) number).

$$\int dF_D = \int -\phi \, dF_A \qquad \because F_A = F_{A0}(1-x).$$

$$F_D - F_{D0} = F_{A0} \int \phi \, dx_A$$

overall yield $\Phi = \dfrac{F_D - F_{D0}}{F_{A0} - F_A}$

$$\Phi = \frac{F_D - F_{D0}}{F_{A0} - F_A} = \frac{F_{A0}}{F_{A0} - F_A} \int \phi \, dx_A$$

$$\Phi = \frac{1}{x_{Af}} \int_0^{x_{Af}} \phi \, dx_A$$

Lets take a CSTR

$\rightarrow F_{D0} - F_D + r_D V = 0$

$\rightarrow F_{A0} - F_A + r_A V = 0$

$\cancel{\phi = F_D}$

$$-\frac{r_D}{r_A} = \frac{F_D - F_{D0}}{F_{A0} - F_A} \; ; \quad -r_A = \frac{F_{A0} X_A}{V}$$

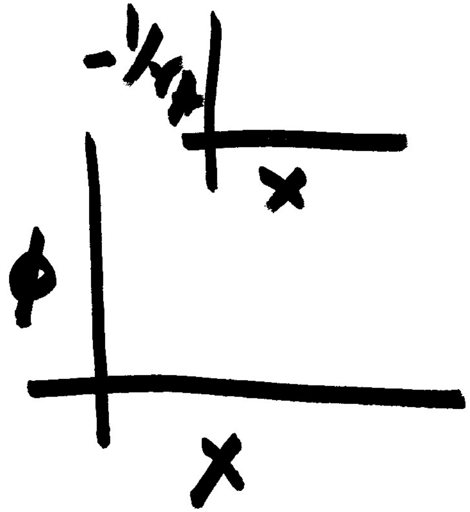
$\phi =$ (def) $\qquad \Phi =$ (Def)

In a CSTR instantaneous yield same as overall yield

Note

1) ϕ, X are measured quantities.

2) $\phi - X$ and $-1/r_A - X$ can be constructed



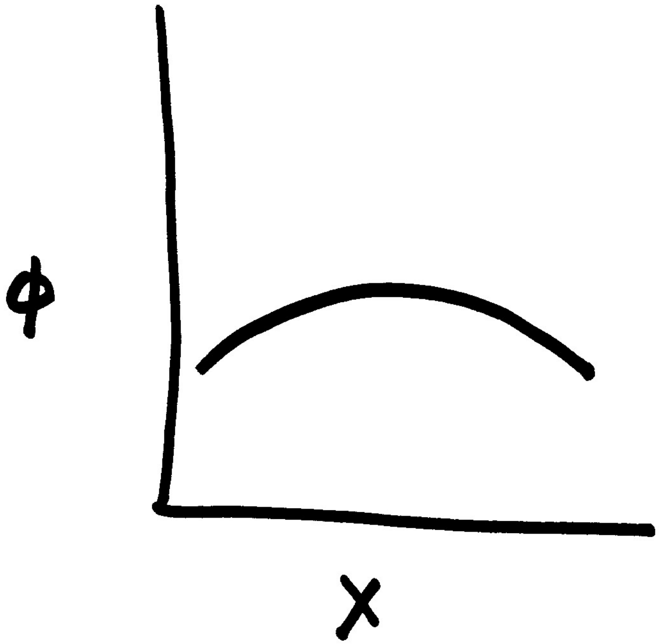


Fig 2

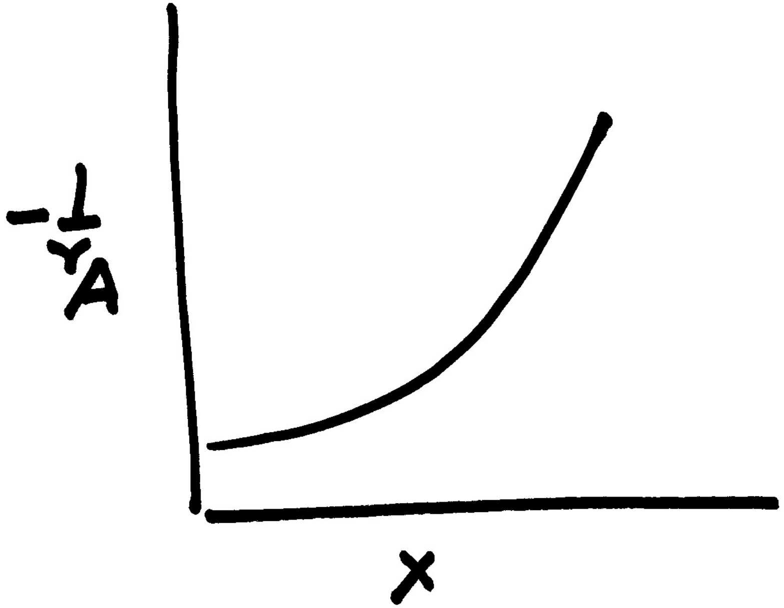
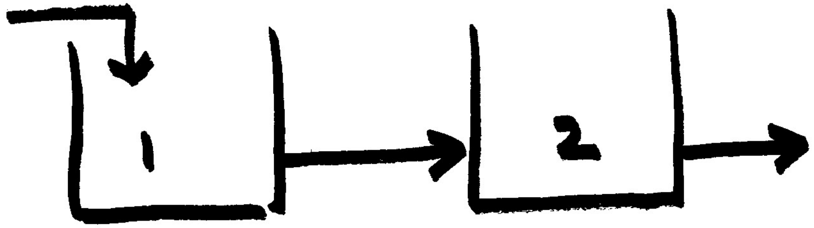


Fig 2

Fig 1 Specifies ϕ ; Fig 2 specifies reactor size.

Combination of Reactors



$$F_{D0} - F_{D1} = -r_{D1} V$$

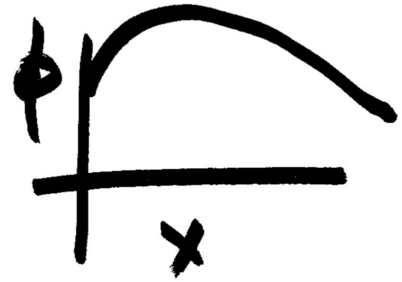
$$F_{A0} - F_{A1} = -r_{A1} V$$

$$\frac{F_{D0} - F_{D1}}{F_{A0} - F_{A1}} = \frac{-r_{D1} V}{-r_{A1} V} = -\phi_1$$

$$F_{D0} - F_{D1} = -\phi_1 F_{A0} X_{A1}$$

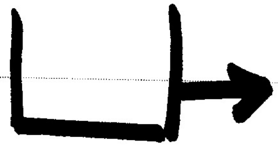
$$\boxed{\Phi_1 =} \quad \frac{F_{D1} - F_{D0}}{F_{A0} - F_{A1}} = \frac{\phi_1 F_{A0} X_{A1}}{F_{A0} X_{A1}} = \phi_1$$

Shows that in single CSTR instantaneous yield ϕ and equal to overall yield



Tank 2

$$F_{D1} - F_{D2} = -r_{D2} V$$



$$F_{A1} - F_{A2} = -r_{A2} V$$

$$\frac{F_{D1} - F_{D2}}{F_{A1} - F_{A2}} = \frac{-r_{D2} V}{-r_{A2} V} = -\phi_2$$

Since $F_{D1} = (\phi_1 F_{A0} X_1 + F_{D0})$ we have

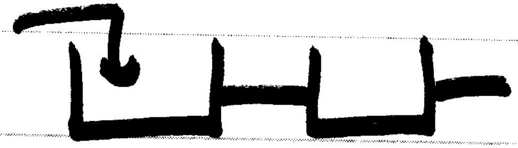
$$(F_{A0} \phi_1 X_1 + F_{D0}) - F_{D2} = -\phi_2 F_{A0} (X_2 - X_1)$$

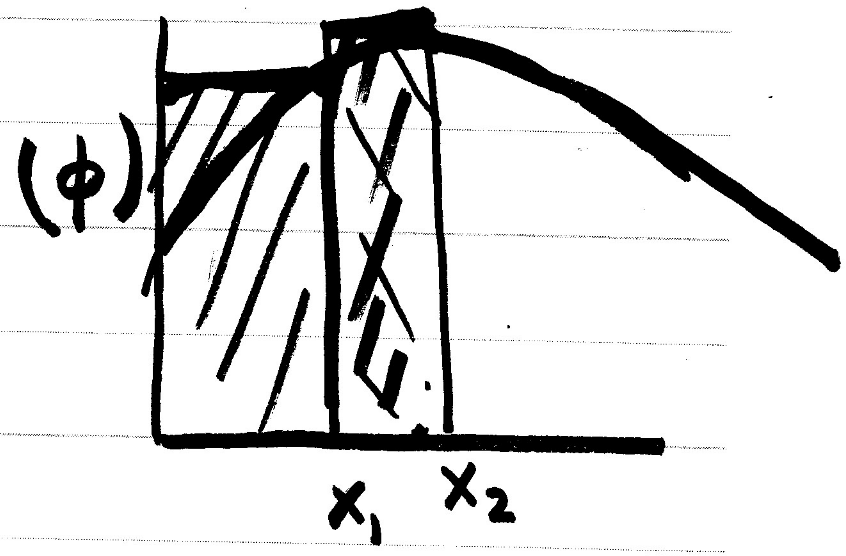
$$\underline{(F_{D2} - F_{D0})} = F_{A0} \phi_1 X_1 + \phi_2 F_{A0} (X_2 - X_1)$$

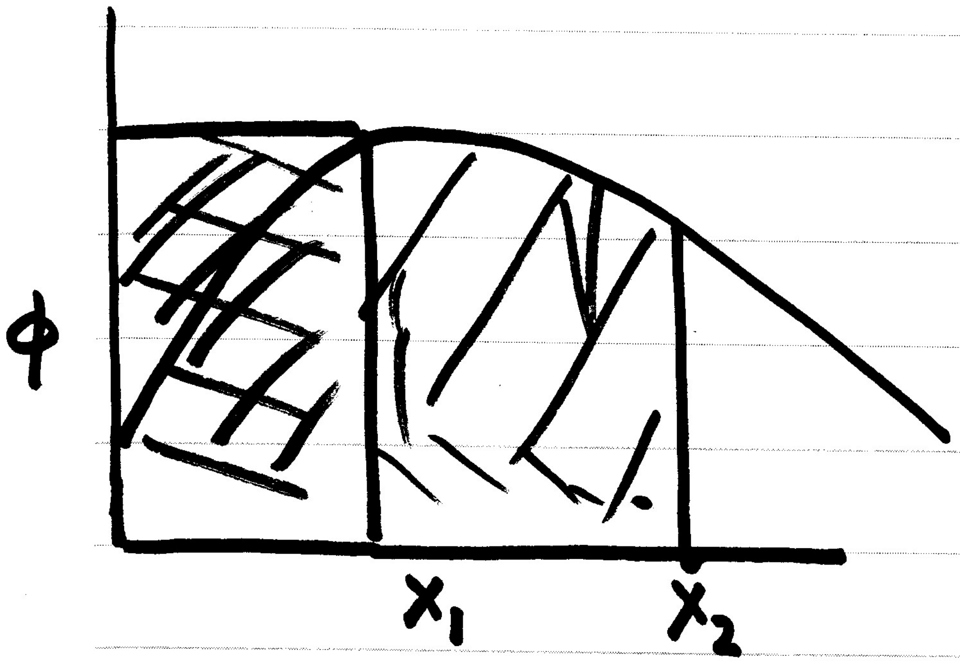
$$\frac{F_{D2}-F_{D0}}{F_{A0}-F_{A2}} = \frac{F_{A0}\,\phi_1 x_1 + \phi_2 F_{A0}(x_2-x_1)}{F_{A0}-F_{A2}}$$

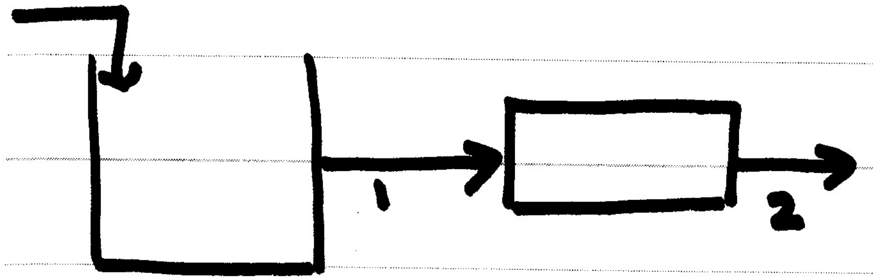
$$\underline{\Phi_2} = \frac{F_{D2}-F_{D0}}{F_{A0}-\underset{?}{F_{A2}}} = \frac{\cancel{F_{A0}}(\phi_1 x_1) + \phi_2 \cancel{F_{A0}}(x_2-x_1)}{\cancel{F_{A0}}\, x_2}$$

$$\Phi_2 = \frac{\phi_1 x_1 + \phi_2 (x_2-x_1)}{x_2}$$

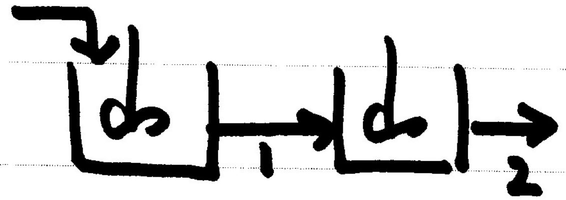


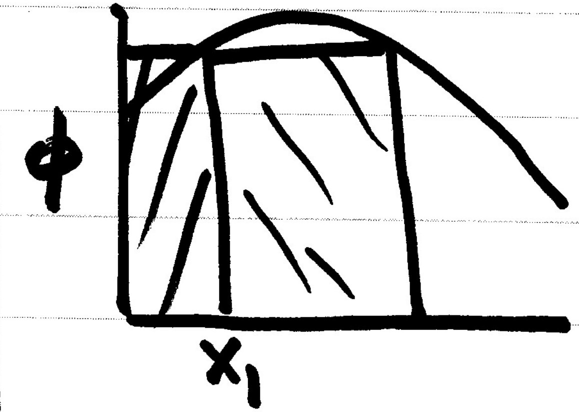




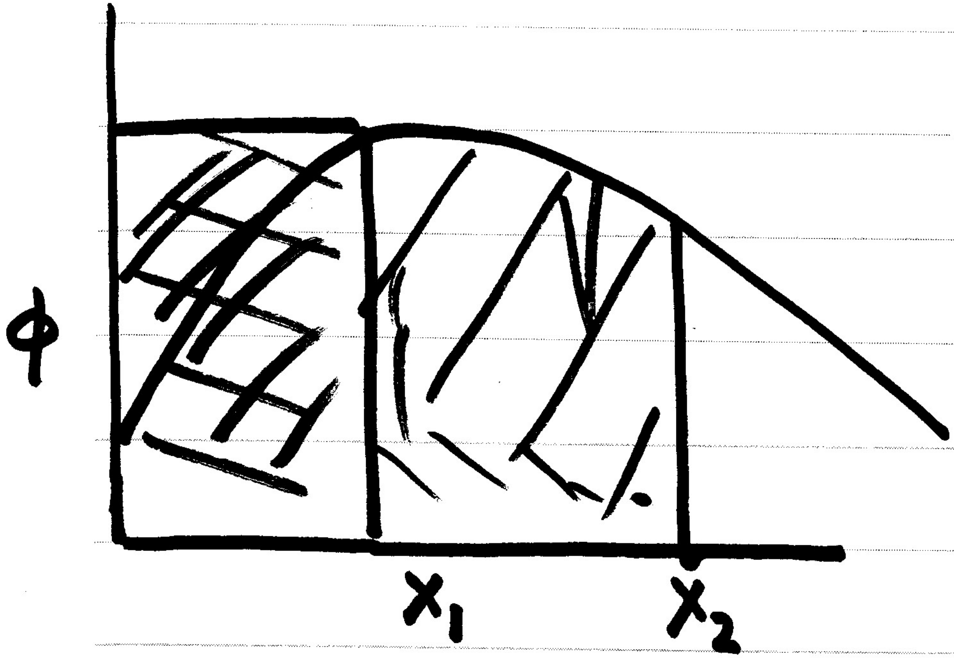


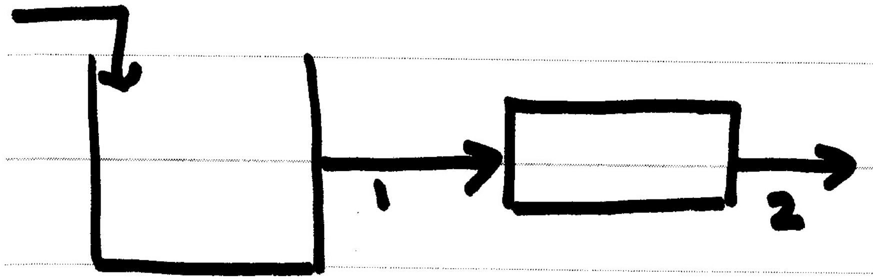
$$\Phi_2 = \frac{\phi_1 x_1 + \int \phi \, dx_A}{x_2}$$



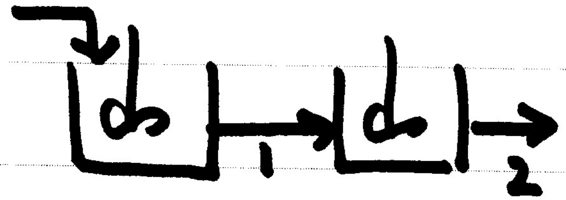


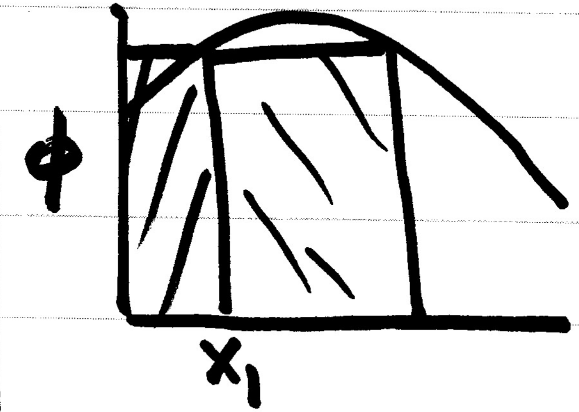
$$\Phi_2 = \frac{\phi_1 x_1 + \phi_2 (x_2 - x_1)}{x_2}$$



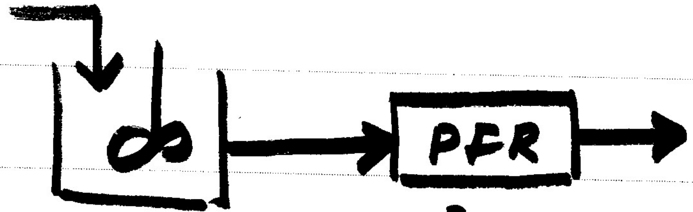


$$\Phi_2 = \frac{\phi_1 x_1 + \int \phi \, d x_A}{x_2}$$





$$\Phi_2 = \frac{\phi_1 x_1 + \phi_2 (x_2 - x_1)}{x_2}$$



1 2

$$\frac{F_{D0}-F_{D1}}{F_{A0}-F_{A1}} = \frac{-r_{D1}}{-r_{A1}} = -\phi_1$$

$$F_{D1}-F_{D0} = \phi_1 F_{A0} x_1$$

$$\frac{dF_D}{dF_A} = \frac{r_D}{r_A} = -\phi$$

$$\int_1^2 dF_D = \int_1^2 -\phi\, dF_A = F_{A0}\int_1^2 \phi\, dx_A$$

$$F_{D2}-F_{D1} = F_{A0}\int_1^2 \phi\, dx_A$$

$$\Phi_2 = \left(\phi_1 x_1 + \int_1^2 \phi\, dx_A\right)/x_2$$

$$F_{D2} - (\phi_1 x_1 F_{A0} + F_{D0}) = F_{A0}\int_1^2 \phi\, dx_A$$

$$F_{D2} - F_{D0} = \phi_1 x_1 F_{A0} + F_{A0}\int_1^2 \phi\, dx_A$$

$$\frac{F_{D2}-F_{D0}}{F_{A0}-F_{A2}} = \Phi_2 = \frac{\phi_1 x_1 F_{A0} + F_{A0}\int_1^2 \phi\, dx_A}{F_{A0}-F_{A2}}$$

Q5

$$\phi = \left(0.6 + 2x - 5x^2\right)$$

The above is experimental data, on a rxn system
ϕ is instantaneous yield
x is conversion

Q5.1 If reaction is to be terminated when ϕ reaches 0.5. What is overall yield in batch reactor. What is overall yield in a CSTR

$\phi = 0.5 \Rightarrow$ what x

Reaction is to be terminated when $\phi = 0.5$

$$0.5 = 0.6 + 2x - 5x^2$$

$$\cancel{x=}\ 0.1 + 2x - 5x^2 = 0$$

$$x = \frac{-2 \pm \sqrt{4 + 2.0}}{-10} = \frac{-2 \pm \sqrt{6}}{10}$$

$$x = 0.447$$

So when x reaches 0.447 stop reaction

$$\Phi(CSTR) = \phi = 0.5$$

In batch reactor

$$\bar{\Phi} : \frac{1}{x} \int_0^x \phi \, dx$$

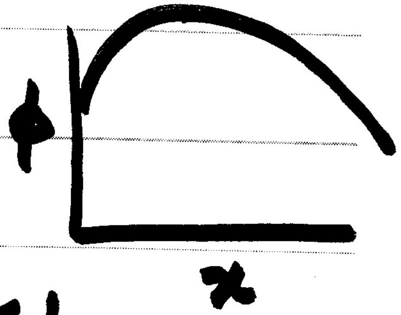
$$\bar{\Phi} : \frac{1}{x} \int_0^x (0.6 + 2x - 5x^2)\, dx$$

$$= \frac{1}{x} \left[0.6x + 2\frac{x^2}{2} - 5\frac{x^3}{3} \right]_0^x$$

$$= \left\{ \frac{1}{x} \left[0.6x + \frac{2x^2}{2} - \frac{5.x^3}{3} \right] \right\}_{x=0.447} = 0.712$$

Q5.2

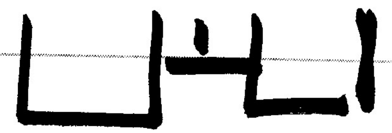
If rxn of Q5.1 is carried out in two tanks in series what conversion in effluent from Tank 1 would lead to highest overall yield



$$x_2 \Phi = \phi_1 x_1 + \phi_2 (x_2 - x_1) \quad ; \quad x_2 \text{ fixed at } 0.447$$

Find x_1 so that Φ is maximised

$$x_2 \frac{d\Phi}{dx_1} = 0 = x_1 \frac{d\phi_1}{dx_1} + \phi_1 - \phi_2$$



Not $\phi = 0.6 + 2x - 5x^2$

So

$$0 = x_1(2 - 10x_1) + (0.6 + 2x_1 - 5x_1^2) - \phi_2$$

$$0 = 2x_1 - 10x_1^2 + 0.6 + 2x_1 - 5x_1^2 - \phi_2$$

$$0 = 4x_1 - 15x_1^2 + 0.1$$

$$x_1 = \frac{-4 \pm \sqrt{16 + 4(0.1)(15)}}{-(2)(15)} \Rightarrow x_1 = 0.286$$

Φ - overall

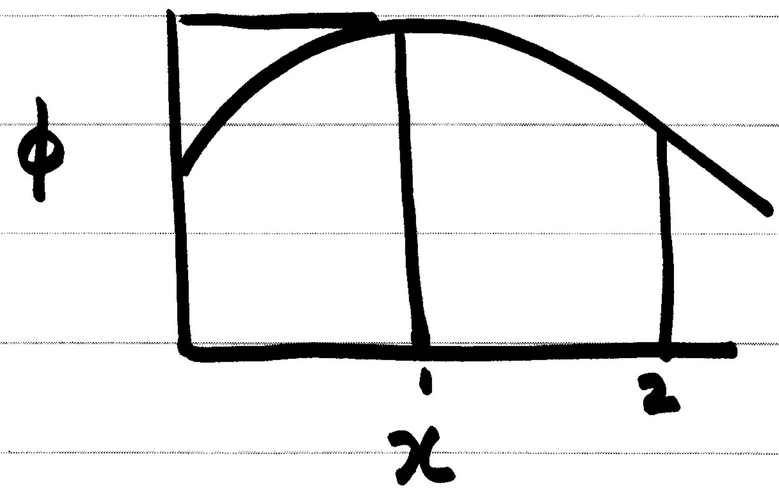
$$\left[\phi_1 x_1 + \phi_2 (x_2 - x_1)\right] / x_2$$

$$\left[0.6 + 2(0.286) - 5(0.286)^2 + 0.5(0.447 - 0.286)\right] / 0.447$$

$$\Phi = 0.669$$

Q5.3

If effluent from plant is to correspond to 50 % conversion what is the highest overall yield which would be obtained. What arrangement would produce it



$\phi = 0.6 + 2x - 5x^2$

max ϕ occurs at

$x = 0.2$

Highest overall yield is obtained by

choosing CSTR followed by PFR

$$\Phi = \frac{\phi_1 x_1 + \int_1^2 \phi \, dx}{x_2}$$

where CSTR works at $x_1 = 0.2$

$$x_2 \quad \Phi = \left[0.6 + 2(0.2) - 5(0.2)^2\right] 0.2$$

$$+ \left(0.6x + \frac{2x^2}{2} - 5\frac{x^3}{3}\right)_{0.2}^{0.5}$$

$$= (0.8)(0.2) + 0.6(0.5 - 0.2) + (0.5^2 - 0.2^2)$$

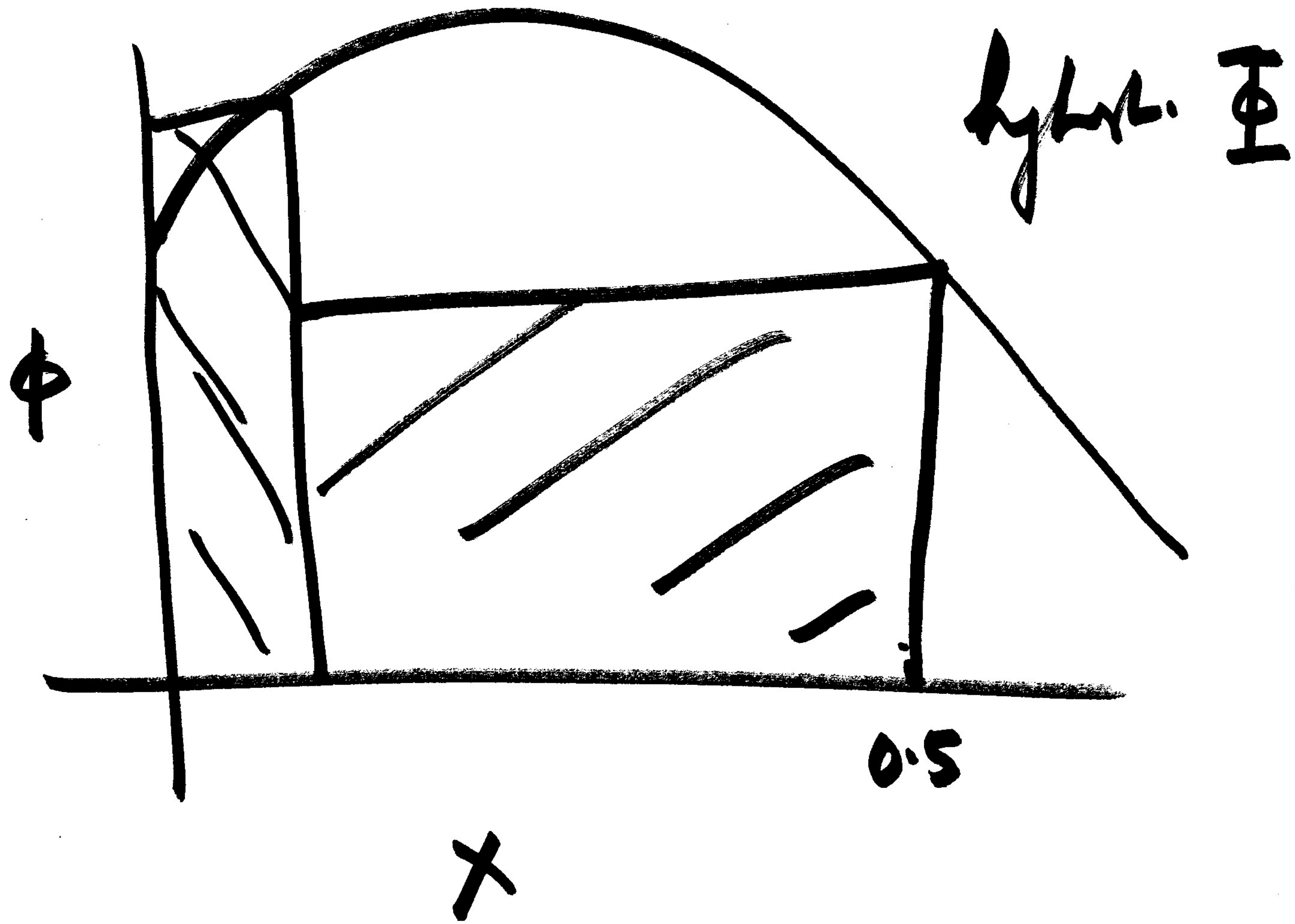
$$- \frac{5}{3}(0.5^3 - 0.2^3)$$

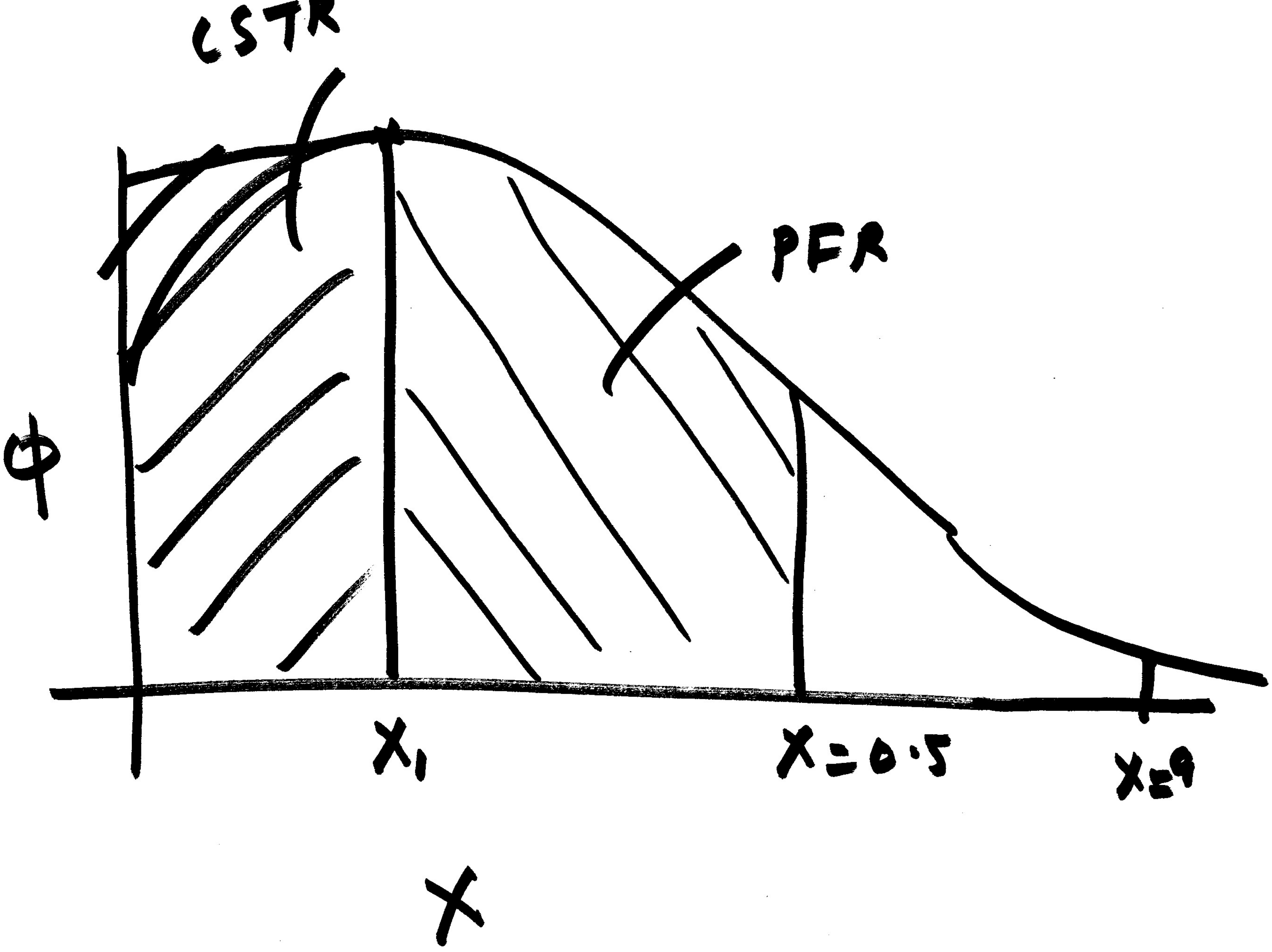
$$= 0.16 + 0.18 + 0.21 - \frac{5}{3}(0.125 - 0.008)$$

$$= 0.16 + 0.18 + 0.21 - 0.195 = 0.355$$

$$\Phi = (0.355)/0.5 = 0.71$$

50 %





CSTR
PFR
Φ
X₁
X=0·5
X=9
X