



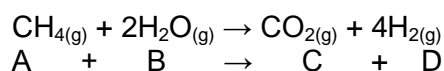
Assignment 1 - Solution

Problem 1

Operating conditions:

- Isobaric
- Isothermal
- Flow reactor
- Ideal gas (*not a great assumption since it is operated at high pressure and temperature*)

a)



→ We know that $y_A = 0.2$; $y_B = 0.7$ and $y_C = 0.1$

→ The limiting reactant is CH_4 since $y_A/v_A < y_B/v_B$ ($0.2 < 0.35$)

Calculate the θ_i values:

$$\theta_A = 1$$

$$\theta_B = \frac{y_B}{y_A} = \frac{0.7}{0.2} = 3.5$$

$$\theta_C = \frac{y_C}{y_A} = \frac{0.1}{0.2} = 0.5$$

Species	Feed	Change	Remaining
A	$\theta_A * F_{A0}$	$-F_{A0} * X$	$F_{A0} * (1-X)$
B	$\theta_B * F_{A0}$	$-(v_B/v_A) F_{A0} * X$	$F_{A0} * (\theta_B - (v_B/v_A) X)$
C	$\theta_C * F_{A0}$	$-(v_C/v_A) F_{A0} * X$	$F_{A0} * (\theta_C - (v_C/v_A) X)$
D	$\theta_D * F_{A0}$	$-(v_D/v_A) F_{A0} * X$	$F_{A0} * (\theta_D - (v_D/v_A) X)$

Species	Feed	Change	Remaining
A	F_{A0}	$-F_{A0} * X$	$F_{A0} * (1-X)$
B	$3.5 * F_{A0}$	$(-2) * F_{A0} * X$	$F_{A0} * (3.5 - (2) * X)$
C	$0.5 * F_{A0}$	$F_{A0} * X$	$F_{A0} * (0.5 + X)$
D	0	$4 * F_{A0} * X$	$F_{A0} * (4) * X$

b)

The equation of a concentration is:

$$C_i = \frac{F_i}{v}$$

For gases, v is not a constant at constant pressure and temperature and it is described by the following formula:

$$v = v_0 (1 + \epsilon X)$$



$$\varepsilon = yA\delta$$

$$\delta = (1 + 4) - (1 + 2) = 2$$

$$\varepsilon = 0.2 * 2 = 0.4 \text{ (not negligible)}$$

$$v_0 = \frac{F_{T0} * R * T_0}{P_0} = 4813.3 \text{ m}^3$$

$$@ X = 0.6$$

$$v = v_0(1 + \varepsilon X) = 4813.3 \text{ m}^3 (1 + 0.4 * 0.6) = 5968.5 \text{ m}^3$$

Concentrations:

Species	Initial (mol/m ³)	Final (mol/m ³)
A	41.55152055	13.40371631
B	145.4303219	77.07136877
C	20.77576028	36.86021984
D	0	80.42229784

c)

The total pressure needs to be constant since it is isobaric.

Since

$$@ X = 0.6$$

The flow rates are:

Species	Initial (kmol/h)	Change (kmol/h)	Remaining (kmol/h)
A	200	-120	80
B	700	-240	460
C	100	120	220
D	0	480	480

$$P_{X=0.6} = \frac{F_T * R * T_0}{v_0(1 + \varepsilon X)}$$

$$P_{X=0.6} = \frac{(80 + 460 + 220 + 480) * 1000 \frac{\text{mol}}{\text{kmol}} * 8.3145 * 1173.15}{4813.3 * (1 + 0.4 * 0.6)} = 2026500 \text{ Pa}$$

which is 20 atm

d)

$$-r_A = k_A C_A C_B^2$$

$$C_A = C_{A0} * \frac{1 - X}{1 + \varepsilon X}$$



$$C_B = C_{A0} * \frac{\theta_B - \left(\frac{v_B}{v_A}\right)X}{1 + \varepsilon X} = C_{A0} \frac{3.5 - 2X}{1 + \varepsilon X}$$

$$-r_A = k_A \left(C_{A0} * \frac{1 - X}{1 + \varepsilon X} \right) \left(C_{A0} \frac{3.5 - 2X}{1 + \varepsilon X} \right)^2$$

$$-r_A = k_A C_{A0}^3 \left(\frac{1 - X}{1 + \varepsilon X} \right) \left(\frac{3.5 - 2X}{1 + \varepsilon X} \right)^2$$

If $k = 1 * 10^{-5} \text{ m}^6/(\text{kmol}^2 \cdot \text{h})$; $X = 0.6$; $\varepsilon = 0.4$ and $C_{A0} = 13.4 \text{ mol/m}^3$

$$-r_A = 7.962 * 10^{-10} \frac{\text{kmol}}{\text{m}^3 \cdot \text{h}}$$

e)

If CO_2 will be removed from the feed while keeping the same total flow rate, temperature and pressure the reaction rate will increase. In other words, R_A increases with an increasing C_A and C_B therefore removing CO_2 from the feed while keeping the same total flow rate will raise the value of C_A and C_B . This will cause the reaction rate to augment (you can also demonstrate it with calculations by changing the initial composition. Consequentially, that will effect the concentration and reaction rate).



Problem 2

$$F_{A0} - F_A + \int r_A dV = \frac{dN_A}{dt}$$

Mass balances for nitrogen (N₂), oxygen (O₂), wood, ash and water.

i) Nitrogen:

$$F_{Nitrogen.0} - F_{Nitrogen} + \int r_{Nitrogen} dV = \frac{dN_{Nitrogen}}{dt}$$

The nitrogen is an inert therefore

F_{i0} and F_i are constant > 0

No reaction: $\int r_{Nitrogen} dV = 0$

No accumulation: $\frac{dN_{Nitrogen}}{dt} = 0$

PFR and CSTR:

$$F_{Nitrogen.0} = F_{Nitrogen}$$

ii) Oxygen:

$$F_{oxygen.0} - F_{oxygen} + \int r_{oxygen} dV = \frac{dN_{oxygen}}{dt}$$

The oxygen is in excess

F_{i0} > 0

F_i > 0

Reaction occurs: $\int r_{oxygen} dV \neq 0$

No accumulation: $\frac{dN_{oxygen}}{dt} = 0$

PFR:

$$F_{oxygen.0} - F_{oxygen} + \int r_{oxygen} dV = 0$$

CSTR:

$$F_{oxygen.0} - F_{oxygen} + r_{oxygen} V = 0$$

iii) Wood:

$$F_{wood.0} - F_{wood} + \int r_{wood} dV = \frac{dN_{wood}}{dt}$$

The wood is fully consumed (X=1)

F_{i0} > 0

F_i = 0

Reaction occurs: $\int r_{wood} dV \neq 0$

No accumulation: $\frac{dN_{wood}}{dt} = 0$

PFR:

$$F_{wood.0} + \int r_{wood} dV = 0$$

CSTR



$$F_{wood.0} + r_{wood}V = 0$$

iv) Ash:

$$F_{Ash.0} - F_{Ash} + \int r_{Ash} dV = \frac{dN_{Ash}}{dt}$$

The ash is only produced and accumulated

$$F_{i0} = 0$$

$$F_i = 0$$

$$\text{Reaction occurs: } \int r_{Ash} dV \neq 0$$

$$\text{No accumulation: } \frac{dN_{Ash}}{dt} \neq 0$$

PFR:

$$\int r_{Ash} dV = \frac{dN_{Ash}}{dt}$$

CSTR:

$$r_{Ash}V = \frac{dN_{Ash}}{dt}$$

v) CO₂:

$$F_{CO2.0} - F_{CO2} + \int r_{CO2} dV = \frac{dN_{CO2}}{dt}$$

The CO₂ is produced

$$F_{i0} = 0$$

$$F_i > 0$$

$$\text{Reaction occurs: } \int r_{CO2} dV \neq 0$$

$$\text{No accumulation: } \frac{dN_{CO2}}{dt} = 0$$

PFR and CSTR:

$$-F_{CO2} + \int r_{CO2} dV = 0$$

vi) Water :

$$F_{water.0} - F_{water} + \int r_{water} dV = \frac{dN_{water}}{dt}$$

Water is in the feed and it is also produced inside the reactor without being accumulated

$$F_{i0} > 0$$

$$F_i > 0$$

$$\text{Reaction occurs: } \int r_{water} dV \neq 0$$

$$\text{No accumulation: } \frac{dN_{water}}{dt} = 0$$

PFR:

$$F_{water.0} - F_{water} + \int r_{water} dV = 0$$

CSTR:

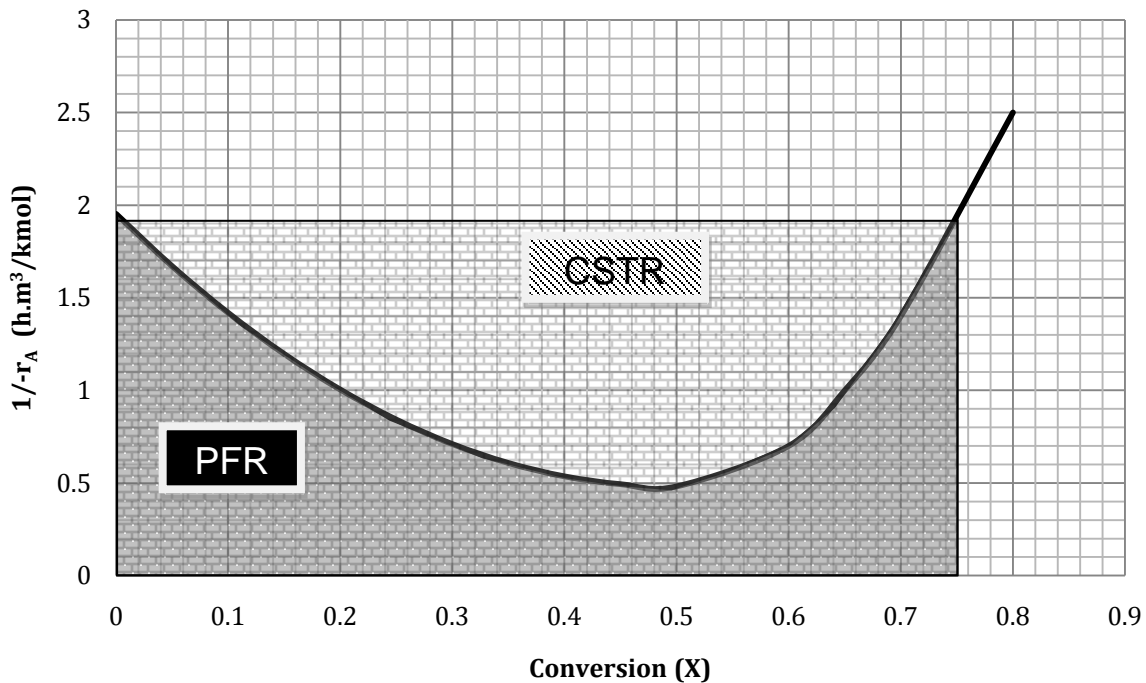
$$F_{water.0} - F_{water} + r_{water}V = 0$$



Problem 3

The area under the curve is proportionate to the PFR volume. The rectangle is proportionate to the CSTR volume. This levenspiel plot graphs $-1/r_A$ in function of X therefore the area determined needs to be multiplied by F_{A0} in order to obtain the reactor volume.

a) For a conversion of $X = 0.75$



From the graph, the volume of the PFR seems to be smaller for a conversion of $X = 0.75$;

Calculation:

@ $X=0.75$, $-1/r_A = 1.92$

For a CSTR:

$$V = X * (F_{A0}/-r_A)$$

$$V = 5.184 \text{ m}^3$$

For a PFR (assume 1 trapezoid):

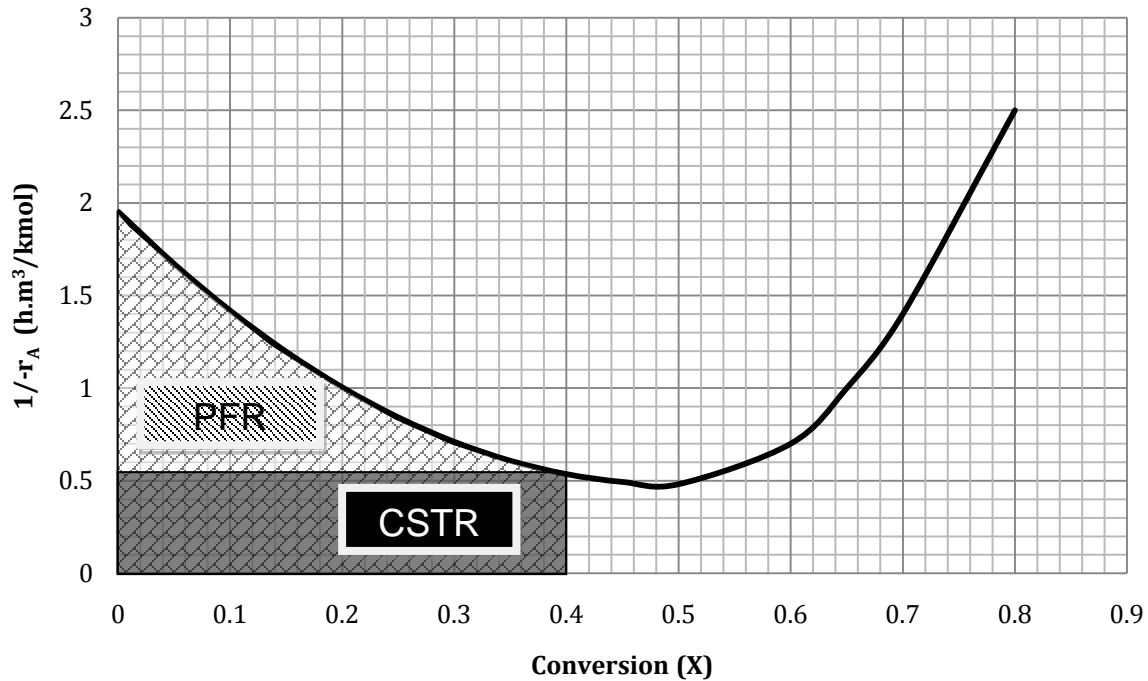
$$V = F_{A0} * \int (-1/r_A) dX$$

$$V = F_{A0} * (((1.95+0.53)*.4/2) + (1.92+0.53)*.35/2)$$

$$V = 3.3291 \text{ m}^3$$



b) For a conversion of $X = 0.4$



From the graph, the volume of the CST seems to be smaller for a conversion of $X = 0.4$;

Calculation:

@ $X=0.4$, $-1/r_A = 0.53$

For CSTR:

$$V = X * (FA_0 / -r_A)$$

$$V = 0.7632 \text{ m}^3$$

For a PFR (assume 2 trapezoids):

$$V = F_{A0} * \int (-1/r_A) dX$$

$$V = FA_0 * ((1.95 + 0.53) * 0.4 / 2)$$

$$V = 1.7856 \text{ m}^3$$

*** I did not provide a detailed calculation of the area under the curve (PFR) in this solution. It is your job know how integrate numerically.



Problem 4:

$$\text{Volume} = 4,000\text{L} = 4 \text{ m}^3$$

Minimum pressure = 1 atm

Maximum pressure = 1.1 atm

Temperature = 20°C

Operating conditions: Batch reactor, isobaric, isothermal, 2 phase reactor

a)

$$F_{A0} - F_A + \int r_A dV = \frac{dN_A}{dt}$$

Constant volume and no flow:

$$r_A V = \frac{dN_A}{dt}$$

If the reaction rate is constant, it is represented by the following equation:

$$-r_A = k_A$$

Therefore:

$$-k_A V = \frac{dN_A}{dt}$$

Since r_A is a constant, k_A is a constant and dN_A/dt is a constant therefore

$$-k_A = \frac{\Delta N_A}{V \cdot \Delta t}$$

It is important to note that r_A is in function of mole therefore $MW_{\text{glucose}} = 0.18 \text{ kg/mol}$

$$-k_A = \frac{\frac{\Delta M_A}{MW_A}}{V \cdot \Delta t}$$

$$k_A = \frac{\frac{20 - 4}{0.18}}{4 * (8 - 0)} = 2.778 \frac{\text{mol}}{\text{m}^3 \cdot \text{h}}$$

Therefore, r_A is:

$$-r_A = k_A = 2.778 \frac{\text{mol}}{\text{m}^3 \cdot \text{h}}$$

b)

Design equation:

$$N_{A0} \frac{dX}{dt} = -r_A V$$



$$t = \frac{N_{A0}\Delta X}{-r_A V} = \frac{\left(\frac{20}{0.18} * (1 - 0)\right)}{(2.778 * 4)} = 10h$$

c)

The pressure increases with increasing conversion. If the reaction was in the liquid phase only , it is reasonable to assume that the pressure is constant but in this case, CO₂ is produced. The gas therefore raises the pressure of the system. Since a pressure relief valve is present, it will not allow the pressure to exceed 1.1 atm. It is important to note that without the pressure relief valve, the system's pressure would keep on rising with increasing conversion which could possibly kill the catalyst (yeast), spoil the sensitive product (wine) or seriously damage the reactor.