



Assignment 2 - Solution

Problem 2

Given:

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

$$v_0 = 200 \text{ L/min}$$

$$C_{A0} = 0.1 \text{ mol/L}$$

$$F_{A0} = C_{A0}v_0 = 0.1 * 200 = 20 \frac{\text{mol}}{\text{min}}$$



$$-r_A = 0.01 (4 C_A - C_B) \text{ [mol/L.min]}$$

a)

$$-r_A = k_A C_A - k_B C_B$$

Therefore, the reaction rate constants k_A and k_B are:

$$k_A = 4 * 0.01 = 0.4 \text{ min}^{-1}$$

$$k_B = 0.01 \text{ min}^{-1}$$

b)

The equilibrium constant is easily calculated in this case since we have both the forward and backward rate constants:

$$K_C = \frac{k_A}{k_B} = \frac{0.4}{0.01} = 4$$

c)

The actual conversion in the reactor is the conversion reached with the given volume. This problem becomes a performance problem.

i) Problem type:
Performance problem

ii) Operating conditions:
CSTR
Liquid phase reaction



Isothermal
Isobaric

iii) Design equation:

$$-r_A = \frac{F_{A0}X}{V}$$

iv) Rate law:

$$-r_A = 0.04 C_A - 0.01 C_B$$

v) Stoichiometry:



$$C_A = C_{A0}(1 - X)$$

$$C_B = C_{A0} \left(\theta_B - \frac{\nu_B}{\nu_A} X \right)$$

vi) Solution:

$$\theta_B = 0$$

Therefore, C_B becomes:

$$C_B = C_{A0}X$$

Combining the concentrations with the reaction rate:

$$-r_A = C_{A0}(0.04(1 - X) - 0.01X) = C_{A0}(0.04 - 0.05X)$$

Combining the rate law and the design equation:

$$C_{A0}(0.04 - 0.05X) = \frac{F_{A0}X}{V}$$

$$X = \frac{0.04}{\frac{F_{A0}}{VC_{A0}} + 0.05}$$

$$X = 0.343$$

d)

The equilibrium conversion occurs when r_A is equal to zero.

$$4C_A = C_B$$

$$C_A = \frac{C_B}{4}$$



$$C_{A0}(1 - X) = \frac{C_{A0}X}{4}$$

$$(1 - X) = \frac{X}{4}$$

$$X = \frac{1}{1.25} = 0.8$$

The equilibrium conversion is at $X = 0.8$.

e)

It is impossible to reach a conversion higher than equilibrium conversion in a CSTR, when the operating conditions are kept constant. If the volume (residence time at a fixed volumetric flow rate) is increased dramatically, the conversion can attain the equilibrium conversion.

The only way to exceed the equilibrium conversion at the stated temperature, pressure and compositions, is by using a membrane PFR or PBR reactor. This type of reactor allows for the removal of product B along the reactor length, causing higher conversions to be reached (Le Chatelier's Principle).

Problem 3

a)

i) Problem type:
Performance problem

ii) Operating conditions:
Isothermal
Non-isobaric (change in pressure)
PBR
Oxygen is the limiting reactant
Gas phase reaction
No limiting reactant since equimolar (we will work as if oxygen was the limiting reactant)

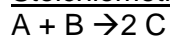
iii) Design equation:
$$\frac{dX}{dW} = -\frac{r'_A}{F_{A0}}$$

iv) Rate law:



$$-r_A' = k_A C_A C_B$$

v) Stoichiometry:



$$C_A = \frac{C_{A0}(1 - X)}{1 + \varepsilon X} y$$

$$C_B = \frac{C_{A0} \left(\theta_B - \frac{\nu_B}{\nu_A} X \right)}{1 + \varepsilon X} y$$

We can calculate the θ_i values

$$\theta_B = 1 \text{ (equimolar)}$$

To find the value of ε

$$\delta = (2) - (1 + 1) = 0$$

$$\varepsilon = y_A \delta = 0$$

Therefore,

$$C_A = C_{A0}(1 - X)y$$

and

$$C_B = C_{A0}(1 - X)y$$

vi) Pressure drop (non-isobaric):

Since $\varepsilon = 0$; the Ergun equation is simplified to,

$$y = (1 - \alpha W)^{\frac{1}{2}}$$

Therefore, the concentrations become the following:

$$C_A = C_{A0}(1 - X)(1 - \alpha W)^{\frac{1}{2}}$$

$$C_B = C_{A0}(1 - X)(1 - \alpha W)^{\frac{1}{2}}$$

vii) Solving:

$$-r_A = k_A C_{A0}(1 - X)(1 - \alpha W)^{\frac{1}{2}} C_{A0}(1 - X)(1 - \alpha W)^{\frac{1}{2}}$$

It becomes:

$$-r_A = k_A C_{A0}^2 (1 - X)^2 (1 - \alpha W)$$

Combining with the design equation:



$$\frac{dX}{dW} = \frac{k_A C_{A0}^2 (1-X)^2 (1-\alpha W)}{F_{A0}}$$

$$\frac{F_{A0}}{k_A C_{A0}^2} \int_{X=0}^X \frac{1}{(1-X)^2} dX = \int_{W=0}^W (1-\alpha W) dW$$

$$\frac{F_{A0}}{k_A C_{A0}^2} \left(\frac{1}{1-X} \right) \Big|_{X=0}^X = W \left(1 - \frac{\alpha}{2} W \right) \Big|_{W=0}^W$$

$$\frac{F_{A0}}{k_A C_{A0}^2} \left(\frac{1}{1-X} \right) - \frac{F_{A0}}{k_A C_{A0}^2} = W \left(1 - \frac{\alpha}{2} W \right)$$

$$\frac{F_{A0}}{k_A C_{A0}^2} \left(\frac{X}{1-X} \right) = W \left(1 - \frac{\alpha}{2} W \right)$$

Consider constants $Y = \frac{F_{A0}}{k_A C_{A0}^2}$ and $Z = W \left(1 - \frac{\alpha}{2} W \right)$

$$Y \left(\frac{X}{1-X} \right) = Z$$

$$X = \frac{Z}{(Y+Z)}$$

$$X = \frac{W \left(1 - \frac{\alpha}{2} W \right)}{\frac{F_{A0}}{k_A C_{A0}^2} + W \left(1 - \frac{\alpha}{2} W \right)}$$

Now to calculate the constants:

$$F_{A0} = 200,000 \frac{\text{mol}}{\text{h}}$$

$$v_0 = 1000 \frac{\text{m}^3}{\text{h}}$$

$$C_{A0} = \frac{F_{A0}}{v_0} = \frac{200,000}{1000} = 200 \frac{\text{mol}}{\text{m}^3}$$

$$k_A = 0.15 \frac{\text{m}^6}{\text{mol.kgcat.h}}$$

Bulk catalyst density:

$$\rho_b = \rho_c (1 - \phi) = 2400 (1 - 0.5) = 1200 \frac{\text{kg}}{\text{m}^3}$$

Catalyst weight:

$$W = A_c \rho_b L = 0.1 * 1200 * 6 = 720 \text{ kg}$$

As proposed earlier,



$$Y = \frac{F_{A0}}{k_A C_{A0}^2} = \frac{200,000}{1.67 * (200^2)} = 33.33$$

Calculating the value of α

$$\alpha = \frac{2\beta_0}{P_0 A_C \rho_b} = \frac{2 * 30}{202.65 * 0.1 * 1200} = 0.002467 \text{ kg}^{-1}$$

Finding the value of Z as proposed earlier,

$$Z = W \left(1 - \frac{\alpha}{2} W \right)$$
$$Z = 720 \left(1 - \frac{0.002467}{2} * 720 \right) = 80.47$$

We can finally find the conversion X,

$$X = \frac{Z}{(Y + Z)} = \frac{80.47}{33.33 + 80.47} = 0.7071$$

b)

If we assume that the reactor is isobaric, $\alpha = 0$. Therefore, Y remains the same while Z becomes:

$$Z = W = 720 \text{ kg}$$

$$X = \frac{Z}{(Y + Z)} = \frac{720}{33.33 + 720} = 0.9558$$

When not considering the pressure drop, the conversion is 0.9558 which is about ~ 0.25 higher than the 0.7071 calculated with pressure drop. It is therefore not wise to assume that the reactor is an isobaric reactor since pressure reduces the conversion by around 25%.