

## Dasar-Dasar Perancangan Reaktor Untuk Reaksi Homogen Isotermal

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Mahasiswa mampu menjelaskan dasar-dasar perancangan reaktor untuk reaksi homogen isotermal

- Penyusunan Persamaan neraca mole secara umum
- Aplikasi neraca mole pada tipe reaktor berbeda: Reaktor batch (RB), reaktor alir tangki berpengaduk (RATB), reaktor alir pipa (RAP), dan reaktor packed bed (RPB).
- Persamaan desain untuk reaksi tunggal RB, RATB, RAP, dan RPB
- Pembahasan contoh soal

### General Mole Balance Equation

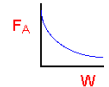
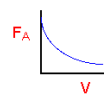
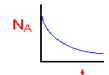
Persamaan neraca mole pada elemen volume  $dV$

$$R_{\text{masuk}} - R_{\text{keluar}} + R_{\text{generasi}} = R_{\text{akumulasi}}$$

$$F_{A0} - F_A + \int_0^V r_A dV = \frac{dN_A}{dt}$$

### Mole Balance on Different Reactor Types

Reactor Type	Differential	Algebraic	Integral
Batch	$\frac{dN_A}{dt} = r_A V$		$t = \int_{N_{A0}}^{N_A} \frac{dN_A}{r_A V}$
CSTR		$V = \frac{F_{A0} - F_A}{-r_A}$	
PFR	$\frac{dF_A}{dV} = r_A$		$V = \int_{F_{A0}}^{F_A} \frac{dF_A}{r_A}$
PBR	$\frac{dF_A}{dW} = r_A'$		$W = \int_{F_{A0}}^{F_A} \frac{dF_A}{r_A'}$



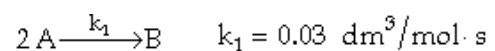
### Case - 01

- Calculate the time to reduce the number of moles by a factor of 10 in a batch reactor for the reaction with  $-r_A = k C_A$ , when  $k = 0.046 \text{ min}^{-1}$



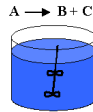
### Case - 02

The irreversible liquid phase second order reaction is carried out in a CSTR. The entering concentration of A,  $C_{A0}$ , is 2 molar and the exit concentration of A,  $C_A$ , is 0.1 molar. The entering and exiting volumetric flow rate,  $v_0$ , is constant at  $3 \text{ dm}^3/\text{s}$ . What is the corresponding reactor volume?



**Case - 03 (CDP1-AA)**

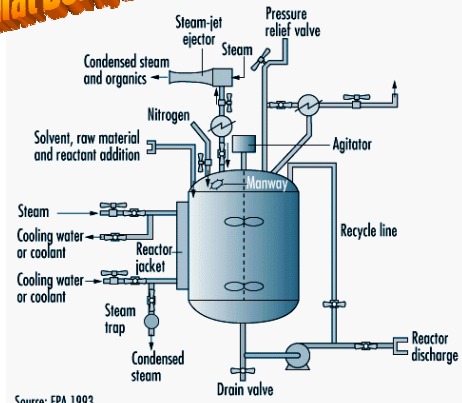
A 200-dm<sup>3</sup> constant-volume batch reactor is pressurized to 20 atm with a mixture of 75% A and 25% inert. The gas-phase reaction is carried out isothermally at 227 °C.



- Assuming that the ideal gas law is valid, how many moles of A are in the reactor initially? What is the initial concentration of A?
- If the reaction is first order:  $-r_A = kC_A$  with  $k = 0.1 \frac{1}{\text{min}}$   
Calculate the time necessary to consume 99% of A.
- If the reaction is second order:  $-r_A = kC_A^2$  with  $k = 0.7 \frac{\text{dm}^3}{\text{mol} \cdot \text{min}}$   
Calculate the time to consume 80% of A. Also calculate the pressure in the reactor at this time if the temperature is 127 °C.

SOLUTION

Selamat Belajar



Source: EPA 1993.

**Solution Case - 01:**

$$t = \int_{N_{A0}}^{N_A} \frac{dN_A}{r_A V} = - \int_{N_{A0}}^{N_A} \frac{dN_A}{-r_A V}$$

$$-r_A V = k C_A V = k \frac{N_A}{V} V = k N_A$$

$$t = \int_{N_A}^{N_{A0}} \frac{dN_A}{k N_A} = \frac{1}{k} \ln \frac{N_{A0}}{N_A}$$

$$t = \frac{1}{0.046 \text{ min}^{-1}} \times \ln 10 = \frac{1}{0.046 \text{ min}^{-1}} \times 2.3$$

Therefore, t = 50 minutes

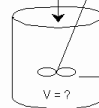
BACK

**Solution Case - 02**

BACK

$$C_{A0} = 2 \text{ mol/dm}^3$$

$$v_0 = 3 \text{ dm}^3/\text{s}$$



$$C_{A0} = 0.1 \text{ mol/dm}^3$$

What is wrong with this solution?

Mole Balance  $V = \frac{F_{A0} - F_A}{-r_A}$

Rate Law  $-r_A = k C_A^2$

Combine  $V = \frac{F_{A0} - F_A}{k C_A^2}$

$$F_{A0} = v_0 C_{A0} = \frac{3 \text{ dm}^3}{\text{s}} \cdot \frac{2 \text{ mol A}}{\text{dm}^3} = \frac{6 \text{ mol A}}{\text{s}}$$

$$F_A = v_0 C_A = \frac{3 \text{ dm}^3}{\text{s}} \cdot \frac{0.1 \text{ mol A}}{\text{dm}^3} = \frac{0.3 \text{ mol A}}{\text{s}}$$

$$V = \frac{(6 - 0.3) \frac{\text{mol}}{\text{s}}}{\left( \frac{0.03 \text{ dm}^3}{\text{mol} \cdot \text{s}} \right) \left( \frac{3 \text{ mol}}{\text{dm}^3} \right)^2} = \frac{5.7 \text{ dm}^3}{0.27} = 21.11 \text{ dm}^3$$

**Solution Case - 03**

- How many moles of A are in the reactor initially? What is the initial concentration of A? If we assume ideal gas behavior, then calculating the moles of A initially present in the reactor is quite simple. We insert our variables into the ideal gas equation:

$$N_{T0} = \frac{P V}{R T} = \frac{20 \text{ atm} \cdot 200 \text{ dm}^3}{0.082 \frac{\text{dm}^3 \cdot \text{atm}}{\text{mol} \cdot \text{K}} \cdot 500 \text{ K}} = 97.6 \text{ mol}$$

Knowing the mole fraction of A ( $y_{A0}$ ) is 75%, we multiply the total number of moles ( $N_{T0}$ ) by the  $y_{A0}$ :

$$N_{A0} = y_{A0} N_{T0} = 73.2 \text{ moles of A}$$

The initial concentration of A ( $C_{A0}$ ) is just the moles of A divided by the volume:

$$C_{A0} = \frac{N_{A0}}{V} = \frac{73 \text{ mol}}{200 \text{ dm}^3} = 0.366 \frac{\text{mol}}{\text{dm}^3}$$

- Time (t) for a 1st order reaction to consume 99% of A. With both 1<sup>st</sup> and 2<sup>nd</sup> order reactions, we will begin with the mole balance:

$$\left[ \begin{array}{c} \text{rate of flow of} \\ \text{species into the} \\ \text{system} \end{array} \right] - \left[ \begin{array}{c} \text{rate of flow of} \\ \text{species out of} \\ \text{the system} \end{array} \right] + \left[ \begin{array}{c} \text{rate of} \\ \text{generation of} \\ \text{species by} \\ \text{reaction in} \\ \text{system} \end{array} \right] = \left[ \begin{array}{c} \text{rate of} \\ \text{accumulation of} \\ \text{species within the} \\ \text{system} \end{array} \right]$$

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

There is no flow in or out of our system, and we will assume that there is no spatial variation in the reaction rate. We are left with:

$$0 - 0 + r_A V = \frac{dN_A}{dt}$$

Knowing the moles per volume ( $N_A/V$ ) is concentration ( $C_A$ ), we then define the reaction rate as a function of concentration:

$$r_A = \frac{dC_A}{dt}$$

### **First Order Reaction**

This is the point where the solutions for the different reaction orders diverge.

Our first order rate law is:  $-r_A = kC_A$

We insert this relation into our mole balance:

$$-kC_A = \frac{dC_A}{dt}$$

and integrate:

$$-k \int dt = \int_{C_{A0}}^{C_A} \frac{dC_A}{C_A}$$

$$-kt = \ln C_A - \ln C_{A0} = \ln \left( \frac{C_A}{C_{A0}} \right)$$

Knowing  $C_A = 0.01 C_{A0}$  and our rate constant ( $k = 0.1 \text{ min}^{-1}$ ), we can solve for the time of the reaction:

$$t = -\frac{1}{k} \ln(0.01) = \frac{4.61}{k} = 46.1 \text{ min}$$

