

**University of Anbar**

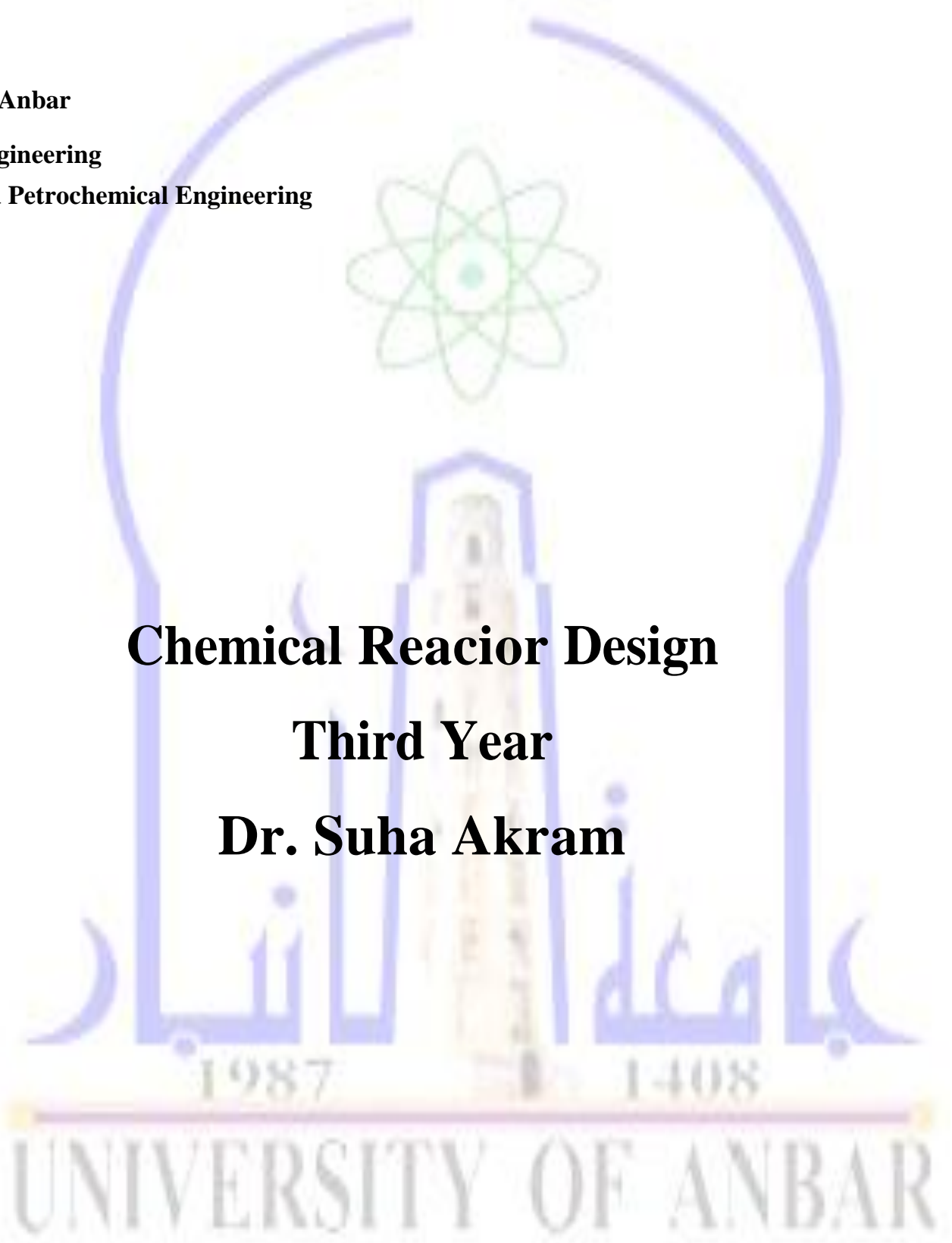
**College of Engineering**

**Chemical and Petrochemical Engineering  
Department**

# **Chemical Reaciior Design**

**Third Year**

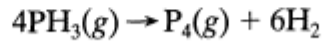
**Dr. Suha Akram**



**Lecture No.9**

**EXAMPLE 5.5 PLUG FLOW REACTOR VOLUME**

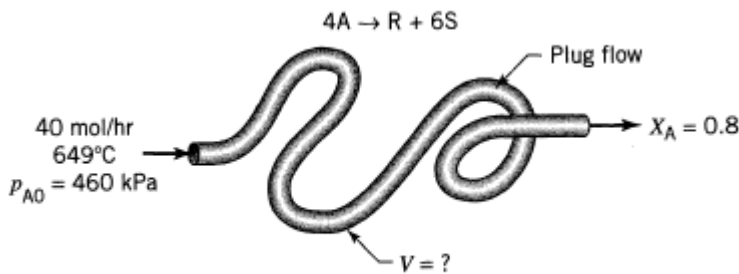
The homogeneous gas decomposition of phosphine



proceeds at 649°C with the first-order rate

$$-r_{\text{PH}_3} = (10/\text{hr}) C_{\text{PH}_3}$$

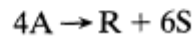
What size of plug flow reactor operating at 649°C and 460 kPa can produce 80% conversion of a feed consisting of 40 mol of pure phosphine per hour?



**Figure E5.5**

**SOLUTION**

Let  $A = \text{PH}_3$ ,  $R = \text{P}_4$ ,  $S = \text{H}_2$ . Then the reaction becomes



With

$$-r_A = (10/\text{hr}) C_A$$

The volume of plug flow reactor is given by Eq. 21

$$V = \frac{F_{A0}}{kC_{A0}} \left[ (1 + \varepsilon_A) \ln \frac{1}{1 - X_A} - \varepsilon_A X_A \right]$$

Evaluating the individual terms in this expression gives

$$F_{A0} = 40 \text{ mol/hr}$$

$$k = 10/\text{hr}$$

$$C_{A0} = \frac{p_{A0}}{RT} = \frac{460\,000 \text{ Pa}}{(8.314 \text{ Pa} \cdot \text{m}^3/\text{mol} \cdot \text{K})(922 \text{ K})} = 60 \text{ mol/m}^3$$

$$\varepsilon_A = \frac{7 - 4}{4} = 0.75$$

$$X_A = 0.8$$

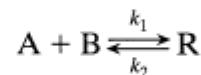
hence the volume of reactor

$$\begin{aligned} V &= \frac{40 \text{ mol/hr}}{(10/\text{hr})(60 \text{ mol/m}^3)} \left[ (1 + 0.75) \ln \frac{1}{0.2} - 0.75(0.8) \right] = 0.148 \text{ m}^3 \\ &= \underline{\underline{148 \text{ liters}}} \end{aligned}$$

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**EXAMPLE 5.6 TEST OF A KINETIC EQUATION IN A PLUG FLOW REACTOR**

We suspect that the gas reaction between A, B, and R is an elementary reversible reaction



and we plan to test this with experiments in an isothermal plug flow reactor.

- (a) Develop the isothermal performance equation for these kinetics for a feed of A, B, R, and inerts.
- (b) Show how to test this equation for an equimolar feed of A and B.

**SOLUTION**

(a) Feed of A, B, R, and inerts. For this elementary reaction the rate is

$$-r_A = k_1 C_A C_B - k_2 C_R = k_1 \frac{N_A}{V} \frac{N_B}{V} - k_2 \frac{N_R}{V}$$

At constant pressure, basing expansion and conversion on substance A,

$$-r_A = k_1 \frac{N_{A0} - N_{A0} X_A}{V_0(1 + \epsilon_A X_A)} \frac{N_{B0} - N_{A0} X_A}{V_0(1 + \epsilon_A X_A)} - k_2 \frac{N_{R0} + N_{A0} X_A}{V_0(1 + \epsilon_A X_A)}$$

Letting  $M = C_{B0}/C_{A0}$ ,  $M' = C_{R0}/C_{A0}$ , we obtain

$$-r_A = k_1 C_{A0}^2 \frac{(1 - X_A)(M - X_A)}{(1 + \epsilon_A X_A)^2} - k_2 C_{A0} \frac{M' + X_A}{1 + \epsilon_A X_A}$$

Hence, the design equation for plug flow, Eq. 17, becomes

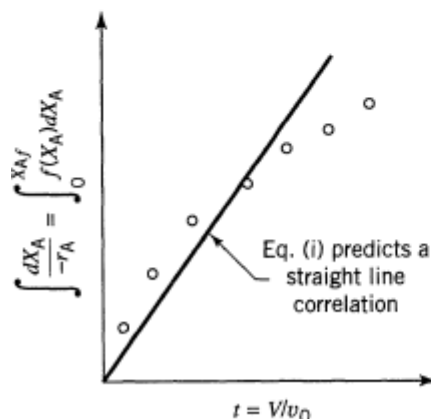
$$\tau = C_{A0} \int_0^{X_{Af}} \frac{dX_A}{-r_A} = \int_0^{X_{Af}} \frac{(1 + \epsilon_A X_A)^2 dX_A}{k_1 C_{A0} (1 - X_A)(M - X_A) - k_2 (M' + X_A)(1 + \epsilon_A X_A)}$$

In this expression  $\epsilon_A$  accounts for the stoichiometry and for inerts present in the feed.

(b) Equimolar feed of A and B. For  $C_{A0} = C_{B0}$ ,  $C_{R0} = 0$ , and no inerts, we have  $M = 1$ ,  $M' = 0$ ,  $\epsilon_A = -0.5$ ; hence the expression for part a reduces to

$$\tau = \int_0^{X_{Af}} \frac{(1 - 0.5X_A)^2 dX_A}{k_1 C_{A0} (1 - X_A)^2 - k_2 X_A (1 - 0.5X_A)} \quad \text{call this } \int_0^{X_{Af}} f(X_A) dX_A \quad \text{(i)}$$

Having  $V$ ,  $v_0$ , and  $X_A$  data from a series of experiments, separately evaluate the left side and the right side of Eq. (i). For the right side, at various  $X_A$



**Figure E5.6**

evaluate  $f(X_A)$ , then integrate graphically to give  $\int f(X_A)dX_A$  and then make the plot of Fig. E5.6. If the data fall on a reasonably straight line, then the suggested kinetic scheme can be said to be satisfactory in that it fits the data.

### Holding Time and Space Time for Flow Reactors

We should be clearly aware of the distinction between these two measures of time,  $\bar{t}$  and  $\tau$ . They are defined as follows:

$$\tau = \left( \begin{array}{l} \text{time needed to} \\ \text{treat one reactor} \\ \text{volume of feed} \end{array} \right) = \frac{V}{v_0} = \frac{C_{A0}V}{F_{A0}}, \quad [\text{hr}] \quad (6) \text{ or } (8)$$

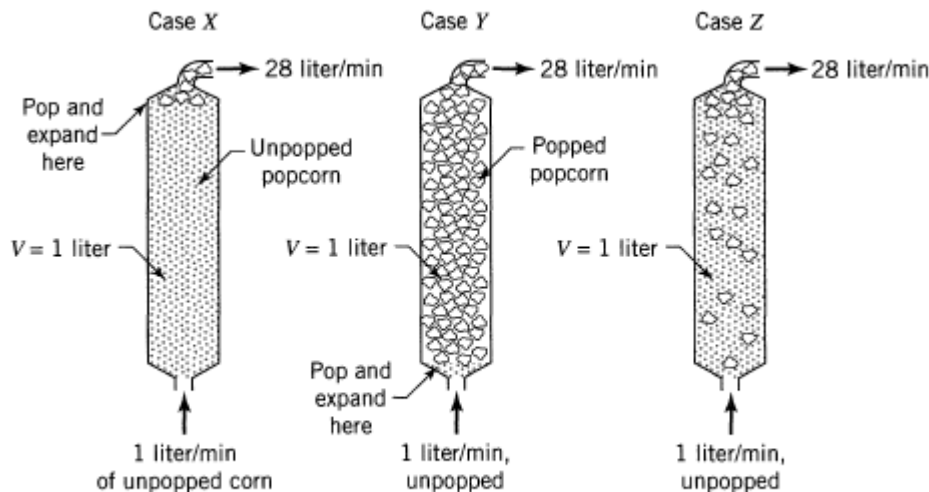
$$\bar{t} = \left( \begin{array}{l} \text{mean residence time} \\ \text{of flowing material} \\ \text{in the reactor} \end{array} \right) = C_{A0} \int_0^{X_A} \frac{dX_A}{(-r_A)(1 + \epsilon_A X_A)}, \quad [\text{hr}] \quad (24)$$

For constant density systems (all liquids and constant density gases)

$$\tau = \bar{t} = \frac{V}{v}$$

For changing density systems  $\bar{t} \neq \tau$  and  $\bar{t} \neq V/v_0$  in which case it becomes difficult to find how these terms are related.

Consider three cases, called X, Y, and Z, which are shown in Fig. 5.7. In the first case (case X) all the popping occurs at the back end of the reactor. In the



**Figure 5.7** For the same  $\tau$  value the  $\bar{t}$  values differ in these three cases.

second case (case Y) all the popping occurs at the front end of the reactor. In the third case (case Z) the popping occurs somewhere between entrance and exit. In all three cases

$$\tau_X = \tau_Y = \tau_Z = \frac{V}{v_0} = \frac{1 \text{ liter}}{1 \text{ liter/min}} = 1 \text{ min}$$

irrespective of where the popping occurs. However, we see that the residence time in the three cases is very different, or

$$\bar{t}_X = \frac{1 \text{ liter}}{1 \text{ liter/min}} = 1 \text{ min}$$

$$\bar{t}_Y = \frac{1 \text{ liter}}{28 \text{ liter/min}} \cong 2 \text{ sec}$$

$\bar{t}_Z$  is somewhere between 2 and 60 s, depending on the kinetics

**Table 5.1** Performance Equations for  $n$ th-order Kinetics and  $\epsilon_A = 0$

|   | Plug Flow or Batch   | Mixed Flow   |
|---|--|--|
| $n = 0$<br>$-r_A = k$                               | $k\tau = \frac{C_{A0} - C_A}{C_{A0}} = X_A$ (20)   | $k\tau = \frac{C_{A0} - C_A}{C_{A0}} = X_A$  |
| $n = 1$<br>$-r_A = kC_A$                            | $k\tau = \ln \frac{C_{A0}}{C_A} = \ln \frac{1}{1 - X_A}$ (3.12)  | $k\tau = \frac{C_{A0} - C_A}{C_A} = \frac{X_A}{1 - X_A}$ (14a)   |
| $n = 2$<br>$-r_A = kC_A^2$                          | $k\tau C_{A0} = \frac{C_{A0} - C_A}{C_A} = \frac{X_A}{1 - X_A}$ (3.16)   | $k\tau = \frac{(C_{A0} - C_A)}{C_A^2} = \frac{X_A}{C_{A0}(1 - X_A)^2}$ (15)                                |
| any $n$<br>$-r_A = kC_A^n$                          | $(n - 1)C_{A0}^{n-1}k\tau = \left(\frac{C_A}{C_{A0}}\right)^{1-n} - 1 = (1 - X_A)^{1-n} - 1$ (3.29)  | $k\tau = \frac{C_{A0} - C_A}{C_A^n} = \frac{X_A}{C_{A0}^{n-1}(1 - X_A)^n}$                                 |
| $n = 1$<br>$A \rightleftharpoons R$<br>$C_{R0} = 0$ | $k_1\tau = \left(1 - \frac{C_{Ar}}{C_{A0}}\right) \ln \left(\frac{C_{A0} - C_{Ar}}{C_A - C_{Ar}}\right) = X_{Ar} \ln \left(\frac{X_{Ar}}{X_{Ar} - X_A}\right)$ | $k_1\tau = \frac{(C_{A0} - C_A)(C_{A0} - C_{Ar})}{C_{A0}(C_A - C_{Ar})} = \frac{X_A X_{Ar}}{X_{Ar} - X_A}$ |
| General rate  | $\tau = \int_{C_A}^{C_{A0}} \frac{dC_A}{-r_A} = C_{A0} \int_0^{X_{Ar}} \frac{dX_A}{-r_A}$ (19)   | $\tau = \frac{C_{A0} - C_A}{-r_A} = \frac{C_{A0} X_A}{-r_A}$ (13)  |