

Montogue

QUIZ CE202 Ideal Reactors – Part 2

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► PROBLEMS

► Problem 1

The reaction



is to be carried out isothermally in a continuous flow reactor. The entering volumetric flow rate v_0 is 10 dm³/h. Calculate both the CSTR and PFR reactor volumes necessary to consume 99% of A (i.e., $C_A = 0.01C_{A,0}$) when the entering molar flow rate is 5 mol/h, assuming the reaction rate $-r_A$ is

$$-r_A = k ; k = 0.05 \frac{\text{mol}}{\text{h} \cdot \text{dm}^3}$$

True or false?

1. () The volume of a CSTR that accommodates this reaction is greater than 100 dm³.
2. () The volume of a PFR that accommodates this reaction is greater than 90 dm³.

Suppose now that the reaction rate is described by

$$-r_A = kC_A ; k = 0.0001 \text{ s}^{-1}$$

3. () The volume of a CSTR that accommodates this reaction is greater than 2600 dm³.
4. () The volume of a PFR that accommodates this reaction is greater than 150 dm³.

Suppose now that the reaction rate is described by

$$-r_A = kC_A^2 ; k = 300 \frac{\text{dm}^3}{\text{mol} \cdot \text{h}}$$

5. () The volume of a CSTR that accommodates this reaction is greater than 700 dm³.
6. () The volume of a PFR that accommodates this reaction is greater than 5 dm³.

► Problem 2

In an isothermal batch reactor, 70% of a liquid reactant is converted in 13 minutes. The reaction, $A \rightarrow R$, is first order on reactant A. What space-time is required to effect this conversion in a plug flow reactor and in a mixed flow reactor? Consider the following statements.

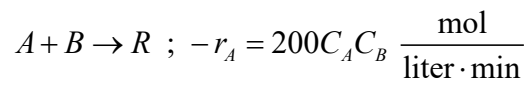
Statement 1: The space-time needed to effect the reaction in a plug flow reactor is greater than 10 minutes.

Statement 2: The space-time needed to effect the reaction in a mixed flow reactor is greater than 30 minutes.

- A) Both statements are true,
- B) Statement 1 is true and statement 2 is false.
- C) Statement 1 is false and statement 2 is true.
- D) Both statements are false.

► Problem 3

An aqueous feed of A and B (400 liter/min, 100 mmol A/liter, 200 mmol B/liter) is to be converted to product in a **mixed flow reactor**. The kinetics of the reaction is represented by

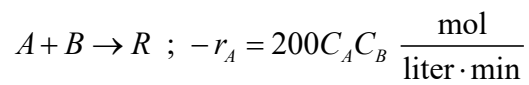


Find the volume of reactor required to for 99.9% conversion of A to product.

- A) $V = 3880$ L
- B) $V = 6540$ L.
- C) $V = 11,100$ L
- D) $V = 20,000$ L

► Problem 4

An aqueous feed of A and B (400 liter/min, 100 mmol A/liter, 200 mmol B/liter) is to be converted to product in a **plug flow reactor**. The kinetics of the reaction are represented by

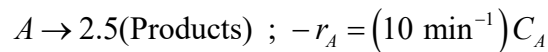


Find the volume of reactor needed for 99.9% conversion of A to product.

- A) $V = 124$ L
- B) $V = 248$ L.
- C) $V = 372$ L
- D) $V = 496$ L

► Problem 5

A gaseous feed of pure A (2 mol/liter, 100 mol/min) decomposes to give a variety of products in a plug flow reactor. The kinetics of the conversion is represented by

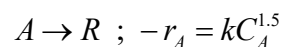


Find the expected conversion in a 22-liter reactor.

- A) $X_A = 0.44$
- B) $X_A = 0.56$
- C) $X_A = 0.71$
- D) $X_A = 0.90$

► Problem 6

We plan to replace our present mixed flow reactor with one having double the volume. For the same aqueous feed (10 mol A/liter) and the same feed rate, find the new conversion. The reaction kinetics are represented by

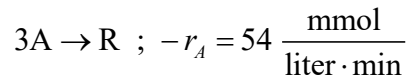


and the present conversion is 70%.

- A) $X'_A = 0.444$
- B) $X'_A = 0.510$
- C) $X'_A = 0.795$
- D) $X'_A = 0.951$

► Problem 7

A stream of pure gaseous reactant A ($C_{A,0} = 660$ mmol/liter) enters a plug flow reactor at a flow rate of $F_{A,0} = 540$ mmol/min and polymerizes there as follows.



How large a reactor is needed to lower the concentration of A in the exit stream to $C_{A,f} = 330$ mmol/liter?

- A) $V = 1.90$ L
- B) $V = 3.81$ L
- C) $V = 7.50$ L
- D) $V = 11.4$ L

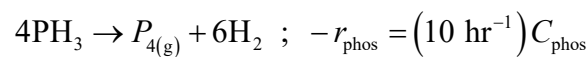
► Problem 8

An aqueous feed containing A (1 mol/liter) enters a 2-liter plug flow reactor and reacts away ($2A \rightarrow R$, $-r_A = 0.05C_A^2$ mol/liter·s). Find the outlet concentration of A for a feed rate of 0.5 liter/min.

- A) $C_{A,f} = 0.0339$ mol/L
- B) $C_{A,f} = 0.0769$ mol/L
- C) $C_{A,f} = 0.112$ mol/L
- D) $C_{A,f} = 0.341$ mol/L

► Problem 9

At 650°C, phosphine vapor decomposes as follows:

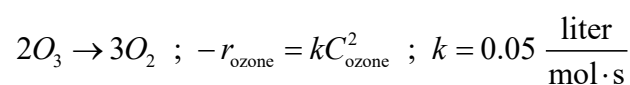


What size of plug flow reactor operating at 649°C and 11.4 atm is needed for 75% conversion of 10 mol/hr of phosphine in a 2/3 phosphine-1/3 inert feed?

- A) $V = 16.9$ L
- B) $V = 31.1$ L
- C) $V = 40.4$ L
- D) $V = 49.2$ L

► Problem 10

1 liter/s of a 20% ozone-80% air mixture at 1.5 atm and 93°C passes through a plug flow reactor. Under these conditions ozone decomposes by the homogeneous reaction

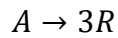


What size reactor is needed for 50% decomposition of ozone?

- A) $V = 1080$ L
- B) $V = 1520$ L
- C) $V = 2130$ L
- D) $V = 2690$ L

► Problem 11

Pure gaseous A at about 3 atm and 30°C (120 mmol/liter) is fed into a 1-liter mixed flow reactor at various flow rates. There it decomposes, and the exit concentration of A is measured for each flow rate. From the following data, find a rate equation to represent the kinetics of the decomposition of A. Assume that reactant A alone affects the rate.



v_0 (liter/min)	0.06	0.48	1.5	8.1
C_A (mmol/liter)	30	60	80	105

- A) $-r_A = 0.002C_A$ mmol/liter·min
- B) $-r_A = 0.004C_A$ mmol/liter·min
- C) $-r_A = 0.002C_A^2$ mmol/liter·min
- D) $-r_A = 0.004C_A^2$ mmol/liter·min

► Problem 12

A mixed flow reactor is being used to determine the kinetics of a reaction whose stoichiometry is $A \rightarrow R$. For this purpose, various flow rates of an aqueous solution of 100 mmol A/liter are fed to a 1-liter reactor, and for each run the outlet concentration of A is measured. Find a rate equation to represent the following data. Also assume that reactant A alone affects the rate.

v (liter/min)	1	6	24
C_A (mmol/liter)	4	20	50

- A) $-r_A = 12C_A$ mmol/liter·min
- B) $-r_A = 24C_A$ mmol/liter·min
- C) $-r_A = 12C_A^2$ mmol/liter·min
- D) $-r_A = 24C_A^2$ mmol/liter·min

→ Problem 13.1

We are planning to operate a batch reactor to convert A into R. This is a liquid reaction, the stoichiometry is $A \rightarrow R$, and the rate of reaction is given in the following table. How long must we react each batch for the concentration to drop from $C_{A,0} = 1.3$ mol/liter to $C_{A,f} = 0.3$ mol/liter?

C_A (mol/liter)	$-r_A$ (mol/liter·min)
0.1	0.1
0.2	0.3
0.3	0.5
0.4	0.6
0.5	0.5
0.6	0.25
0.7	0.10
0.8	0.06
1.0	0.05
1.3	0.045
2.0	0.042

- A) $t = 8.41$ min
- B) $t = 12.7$ min
- C) $t = 19.4$ min
- D) $t = 23.2$ min

→ Problem 13.2

For the reaction in the previous problem, what size of plug flow reactor would be needed for 80% conversion of a feed stream of 1000 mol A/hr at $C_{A,0} = 1.5$ mol/liter?

- A) $V = 70.9$ L
- B) $V = 110$ L
- C) $V = 191$ L
- D) $V = 275$ L

► Problem 14

The data in the following table have been obtained on the decomposition of gaseous reactant A in a constant volume batch reactor at 100°C. The stoichiometry of the reaction is $2A \rightarrow R + S$. What size mixed flow reactor operating at 100°C and 1 atm can treat 100 mol A/hr in a feed consisting of 20% inerts to obtain 95% conversion of A?

t (sec)	p_A (atm)	t (sec)	p_A (atm)
0	1.0	140	0.25
20	0.80	200	0.14
40	0.68	260	0.08
60	0.56	330	0.04
80	0.45	420	0.02
100	0.37		

- A) $V = 585$ L
 B) $V = 1050$ L
 C) $V = 1540$ L
 D) $V = 2160$ L

► ADDITIONAL INFORMATION

Table 1 Performance equations for n -th order kinetics and $\varepsilon_A = 0$

	Plug Flow or Batch	Mixed Flow
$n = 0$ $-r_A = k$	$\frac{k\tau}{C_{A0}} = \frac{C_{A0} - C_A}{C_{A0}} = X_A \quad (20)$	$\frac{k\tau}{C_{A0}} = \frac{C_{A0} - C_A}{C_{A0}} = X_A$
$n = 1$ $-r_A = kC_A$	$k\tau = \ln \frac{C_{A0}}{C_A} = \ln \frac{1}{1 - X_A} \quad (3.12)$	$k\tau = \frac{C_{A0} - C_A}{C_A} = \frac{X_A}{1 - X_A} \quad (14a)$
$n = 2$ $-r_A = kC_A^2$	$k\tau C_{A0} = \frac{C_{A0} - C_A}{C_A} = \frac{X_A}{1 - X_A} \quad (3.16)$	$k\tau = \frac{(C_{A0} - C_A)}{C_A^2} = \frac{X_A}{C_{A0}(1 - X_A)^2} \quad (15)$
any n $-r_A = kC_A^n$	$(n - 1)C_{A0}^{n-1}k\tau = \left(\frac{C_A}{C_{A0}}\right)^{1-n} - 1 = (1 - X_A)^{1-n} - 1 \quad (3.29)$	$k\tau = \frac{C_{A0} - C_A}{C_A^n} = \frac{X_A}{C_{A0}^{n-1}(1 - X_A)^n}$
$n = 1$ $A \xrightleftharpoons[2]{1} R$ $C_{R0} = 0$	$k_1\tau = \left(1 - \frac{C_{Ae}}{C_{A0}}\right) \ln \left(\frac{C_{A0} - C_{Ae}}{C_A - C_{Ae}}\right) = X_{Ae} \ln \left(\frac{X_{Ae}}{X_{Ae} - X_A}\right)$	$k_1\tau = \frac{(C_{A0} - C_A)(C_{A0} - C_{Ae})}{C_{A0}(C_A - C_{Ae})} = \frac{X_A X_{Ae}}{X_{Ae} - X_A}$
General rate	$\tau = \int_{C_A}^{C_{A0}} \frac{dC_A}{-r_A} = C_{A0} \int_0^{X_{Ae}} \frac{dX_A}{-r_A} \quad (19)$	$\tau = \frac{C_{A0} - C_A}{-r_{Af}} = \frac{C_{A0} X_A}{-r_{Af}} \quad (13)$

Table 2 Performance equations for n -th order kinetics and $\varepsilon_A \neq 0$

	Plug Flow	Mixed Flow
$n = 0$ $-r_A = k$	$\frac{k\tau}{C_{A0}} = X_A$ (20)	$\frac{k\tau}{C_{A0}} = X_A$
$n = 1$ $-r_A = kC_A$	$k\tau = (1 + \varepsilon_A) \ln \frac{1}{1 - X_A} - \varepsilon_A X_A$ (21)	$k\tau = \frac{X_A(1 + \varepsilon_A X_A)}{1 - X_A}$ (14b)
$n = 2$ $-r_A = kC_A^2$	$k\tau C_{A0} = 2\varepsilon_A(1 + \varepsilon_A) \ln(1 - X_A) + \varepsilon_A^2 X_A + (\varepsilon_A + 1)^2 \cdot \frac{X_A}{1 - X_A}$ (23)	$k\tau C_{A0} = \frac{X_A(1 + \varepsilon_A X_A)^2}{(1 - X_A)^2}$ (15)
any n $-r_A = kC_A^n$		$k\tau C_{A0}^{n-1} = \frac{X_A(1 + \varepsilon_A X_A)^n}{(1 - X_A)^n}$
$n = 1$ $A \xrightleftharpoons[2]{1} rR$ $C_{R0} = 0$	$\frac{k\tau}{X_{Ae}} = (1 + \varepsilon_A X_{Ae}) \ln \frac{X_{Ae}}{X_{Ae} - X_A} - \varepsilon_A X_A$ (22)	$\frac{k\tau}{X_{Ae}} = \frac{X_A(1 + \varepsilon_A X_A)}{X_{Ae} - X_A}$
General expression	$\tau = C_{A0} \int_0^{X_A} \frac{dX_A}{-r_A}$ (17)	$\tau = \frac{C_{A0} X_A}{-r_A}$ (11)

➤ SOLUTIONS

P.1 ➔ Solution

1. **False.** The design equation for the CSTR is

$$V = \frac{F_{A,0} - F_A}{-r_A}$$

$$\therefore V = \frac{C_{A,0}v_0 - C_A v_0}{-r_A}$$

so that

$$V = \frac{C_{A,0}v_0 - C_A v_0}{-r_A} = \frac{0.5 \times 10 - (0.01 \times 0.5) \times 10}{0.05} = \boxed{99 \text{ dm}^3}$$

2. True. Consider now the PFR under the same conditions. The reaction is modeled as

$$\begin{aligned}
 -v_0 \frac{dC_A}{dV} &= k \rightarrow -\frac{v_0}{k} dC_A = dV \\
 \therefore \int_0^V dV &= -\frac{v_0}{k} \int_{C_{A,0}}^{C_A} dC_A \\
 \therefore V &= -\frac{v_0}{k} (C_A - C_{A,0})
 \end{aligned}$$

Substituting the numerical quantities brings to

$$V = -\frac{10}{0.05} \times (0.01 \times 0.5 - 0.5) = \boxed{99 \text{ dm}^3}$$

3. True. With the rate of reaction $-r_A = kC_A$, the CSTR volume becomes

$$V = \frac{C_{A,0}v_0 - C_A v_0}{kC_A} = \frac{1 \text{ h}}{3600 \text{ s}} \times \left(\frac{0.5 \times 10 - 0.01 \times 0.5 \times 10}{0.0001 \times 0.01 \times 0.5} \right) = \boxed{2750 \text{ dm}^3}$$

4. False. We proceed to consider the PFR under the same conditions. The reaction is modeled as

$$\begin{aligned}
 -v_0 \frac{dC_A}{dV} &= kC_A \rightarrow \frac{v_0}{k} \frac{dC_A}{C_A} = \int_0^V dV \\
 \therefore V &= -\frac{v_0}{k} \ln \left(\frac{C_A}{C_{A,0}} \right)
 \end{aligned}$$

Substituting the numerical quantities, we obtain

$$V = -\frac{1 \text{ h}}{3600 \text{ s}} \times \frac{10}{0.0001} \times \ln \left(\frac{0.01 \times 0.5}{0.5} \right) = \boxed{128 \text{ dm}^3}$$

5. False. With the rate of reaction $-r_A = kC_A^2$, the CSTR volume becomes

$$V = \frac{C_{A,0}v_0 - C_A v_0}{kC_A^2} = \frac{0.5 \times 10 - 0.01 \times 0.5 \times 10}{300 \times (0.01 \times 0.5)^2} = \boxed{660 \text{ dm}^3}$$

6. True. We proceed to consider the PFR under the same conditions. The reaction is modeled as

$$\begin{aligned}
 -v_0 \frac{dC_A}{dV} &= kC_A^2 \rightarrow -\frac{v_0}{k} \int_{C_{A,0}}^{C_A} \frac{dC_A}{C_A^2} = \int_0^V dV \\
 \therefore V &= \frac{v_0}{k} \left(\frac{1}{C_A} - \frac{1}{C_{A,0}} \right)
 \end{aligned}$$

Substituting the numerical quantities, we get

$$V = \frac{10}{300} \times \left(\frac{1}{0.01 \times 0.5} - \frac{1}{0.5} \right) = \boxed{6.6 \text{ dm}^3}$$

P.2 → Solution

In the batch reactor, 70% conversion occurs in 13 min. Thus, the holding time or mean residence time in the batch reactor is 13 min. For a constant fluid density system, the space time is equivalent to the holding time of the reactor. In a plug flow reactor, the space time required would be the same as the holding time in the batch reactor; accordingly, we surmise that the space time for the plug flow reactor to achieve 70% conversion is equal to 13 minutes.

Consider now the same reaction being carried out in a mixed flow reactor. For a first order reaction, the rate expression is $r_A = kC_A$. Substituting in the performance equation brings to

$$t = -\int_0^{X_{A,f}} \frac{dX_A}{-r_A} = \int_0^{X_{A,f}} \frac{dX_A}{kC_{A,0}(1-X_A)} = -\frac{\ln(1-X_A)}{k}$$

$$\therefore k = -\frac{\ln(1 - X_A)}{t}$$

$$\therefore k = -\frac{\ln(1 - 0.7)}{13} = 0.0926 \text{ min}^{-1}$$

Equipped with the rate constant, we can determine the space time τ ,

$$\frac{\tau}{C_{A,0}} = \frac{X_A}{-r_A} \rightarrow \tau = \frac{C_{A,0} X_A}{k C_A}$$

$$\therefore \tau = \frac{\cancel{C_{A,0}} X_A}{k \cancel{C_{A,0}} (1 - X_A)}$$

$$\therefore \tau = \frac{X_A}{k(1 - X_A)}$$

$$\therefore \tau = \frac{0.7}{0.0926 \times (1 - 0.7)} = 25.2 \text{ min}$$

◆ The correct answer is **B**.

P.3 → Solution

The rate equation for the reaction can be rewritten as

$$-r_A = 200(C_{A,0} - C_{A,0} X_A)(C_{B,0} - C_{B,0} X_A)$$

Taking $M = C_{B,0}/C_{A,0} = 200/100 = 2.0$ as the initial molar ratio of reactants, we have

$$-r_A = 200 C_{A,0}^2 (1 - X_A)(M - X_A) \frac{\text{mol}}{\text{liter} \cdot \text{min}}$$

The space time τ is given by

$$\tau = \frac{C_{A,0} X_A}{-r_A}$$

Since $\tau = V/v_0$, we have

$$\frac{V}{v_0} = \frac{C_{A,0} X_A}{-r_A} \rightarrow V = \frac{v_0 C_{A,0} X_A}{-r_A}$$

Finally, we substitute our data to obtain

$$V = \frac{v_0 C_{A,0} X_A}{-r_A} \rightarrow V = \frac{v_0 C_{A,0} X_A}{200 C_{A,0}^2 (1 - X_A)(M - X_A)}$$

$$\therefore V = \frac{v_0 X_A}{200 C_{A,0} (1 - X_A)(M - X_A)}$$

$$\therefore V = \frac{400 \times 0.999}{200 \times (100/1000) \times (1 - 0.999) \times (2 - 0.999)} = \boxed{20,000 \text{ L}}$$

◆ The correct answer is **D**.

P.4 → Solution

For a second-order reaction such as the present one, we have

$$k\tau C_{A,0} (M - 1) = \ln \left[\frac{M - X_A}{M(1 - X_A)} \right]$$

where the initial molar ratio of reactants $M = C_{B,0}/C_{A,0} = 200/100 = 2.0$. Inserting this and other data in the equation gives

$$200 \times \tau \times 0.1 \times (2 - 1) = \ln \left[\frac{2 - 0.999}{2 \times (1 - 0.999)} \right]$$

$$\therefore 20\tau = 6.22$$

$$\therefore \tau = 0.311 \text{ min}$$

The reactor volume required is determined to be

$$V = \tau v = 0.311 \times 400 = \boxed{124 \text{ L}}$$

◆ The correct answer is **A**.

P.5 → Solution

The expansion factor is $\varepsilon_A = (2.5 - 1.0)/1.0 = 1.5$. The performance equation for a first-order reaction with $\varepsilon_A \neq 0$ is given by equation (21) of Table 2,

$$k\tau = (1 + \varepsilon_A) \ln\left(\frac{1}{1 - X_A}\right) - \varepsilon_A X_A$$

Substituting $\tau = VC_{A,0}/F_{A,0}$ gives

$$\frac{kVC_{A,0}}{F_{A,0}} = (1 + \varepsilon_A) \ln\left(\frac{1}{1 - X_A}\right) - \varepsilon_A X_A$$

Inserting the numerical data, we have

$$\frac{10 \times 22 \times 2}{100} = (1 + 1.5) \ln\left(\frac{1}{1 - X_A}\right) - 1.5 X_A$$

$$\therefore 4.4 = 2.5 \ln\left(\frac{1}{1 - X_A}\right) - 1.5 X_A$$

The result above is a nonlinear equation in X_A . One way to solve it is to apply the *FindRoot* command in Mathematica, using an initial guess of $X_A = 0.5$,

$$\text{FindRoot}[4.4 - 2.5\text{Log}[1/(1 - x_A)] + 1.5x_A, \{x_A, 0.5\}]$$

The code above returns $X_A = 0.90$. Thus, the conversion in the plug flow reactor is about 90%.

◆ The correct answer is **D**.

P.6 → Solution

The performance equation for the reactor is

$$\frac{V}{F_{A,0}} = \frac{X_A}{-r_A}$$

which, substituting the relation we have for r_A , becomes

$$\frac{V}{F_{A,0}} = \frac{X_A}{-r_A} \rightarrow \frac{V}{F_{A,0}} = \frac{X_A}{kC_{A,0}^{1.5}(1 - X_A)^{1.5}}$$

$$\therefore \frac{Vk}{F_{A,0}} = \frac{X_A}{C_{A,0}^{1.5}(1 - X_A)^{1.5}}$$

Inserting $C_{A,0} = 10 \text{ mol/L}$ and $X_A = 0.7$ in the right-hand side gives

$$\frac{Vk}{F_{A,0}} = \frac{0.7}{10^{1.5} \times (1 - 0.7)^{1.5}} = 0.135 \text{ (I)}$$

Now, suppose we had a mixed flow reactor with twice the volume of the original. We restate the performance equation as

$$\frac{2V}{F_{A,0}} = \frac{X'_A}{kC_{A,0}^{1.5}(1 - X'_A)^{1.5}} \rightarrow 2\left(\frac{Vk}{F_{A,0}}\right) = \frac{X'_A}{10^{1.5}(1 - X'_A)^{1.5}}$$

$$\therefore 2\left(\frac{Vk}{F_{A,0}}\right) = \frac{X'_A}{31.6(1 - X'_A)^{1.5}}$$

From equation (I), we know that the term in parentheses in the left-hand side equals 0.135. Substituting and squaring both sides, we obtain

$$2 \times \left(\frac{Vk}{F_{A,0}} \right) = \frac{X'_A}{31.6(1-X'_A)^{1.5}} \rightarrow 2 \times 0.135 = \frac{X'_A}{C_{A,0}^{1.5}(1-X'_A)^{1.5}}$$

$$\therefore 0.27 = \frac{X'_A}{31.6(1-X'_A)^{1.5}}$$

$$\therefore (0.27 \times 31.6)^2 = \left[\frac{X'_A}{(1-X'_A)^{1.5}} \right]^2$$

$$\therefore 72.8 = \frac{X'^2_A}{(1-X'_A)^3}$$

The result above is a third-degree equation in X'_A , which can be expanded to give

$$-72.8X'^3_A + 217.4X'^2_A - 218.4X'_A + 72.8 = 0$$

One way to solve this equation is to employ Mathematica's *Solve* command, using the following syntax,

$$\text{Solve}[-72.8x^3 + 217.4x^2 - 218.4x + 72.8 == 0, x]$$

This returns $x = X'_A = 0.795$. The conversion of the larger reactor is about 79.5%.

◆ The correct answer is **C**.

P.7 → Solution

The expansion factor is $\varepsilon_A = (1 - 3)/3 = -0.667$. From the expression for r_A , it is easy to see that the reaction in question is a zero order reaction. In this case, the pertinent performance equation is

$$\frac{k\tau}{C_{A,0}} = \frac{kV}{F_{A,0}} = X_{A,f} \rightarrow V = \frac{F_{A,0}X_{A,f}}{k} \quad (\text{I})$$

The final concentration of reactant is given by

$$\frac{C_{A,f}}{C_{A,0}} = \frac{1 - X_{A,f}}{1 + \varepsilon_A X_{A,f}}$$

Substituting $C_{A,0} = 660$ mmol/L, $C_{A,f} = 330$ mmol/L, and $\varepsilon_A = -0.667$, we have

$$\frac{330}{660} = \frac{1 - X_{A,f}}{1 - 0.667X_{A,f}} \rightarrow X_{A,f} = 0.750$$

Substituting this and other data into equation (I) gives

$$V = \frac{540 \times 0.750}{54} = \boxed{7.5 \text{ L}}$$

◆ The correct answer is **C**.

P.8 → Solution

From the expression we were given for r_A , it is easy to conclude that the reaction is a second-order reaction. The appropriate performance equation is then

$$k\tau C_{A,0} = \frac{C_{A,0} - C_{A,f}}{C_{A,f}}$$

Substituting $\tau = V/v_0$ and solving for $C_{A,f}$, we get

$$k\tau C_{A,0} = \frac{C_{A,0} - C_{A,f}}{C_{A,f}} \rightarrow k \frac{V}{v_0} C_{A,0} = \frac{C_{A,0} - C_{A,f}}{C_{A,f}}$$

$$\therefore k \frac{V}{v_0} C_{A,0} = \frac{C_{A,0}}{C_{A,f}} - 1$$

$$\therefore \frac{C_{A,0}}{C_{A,f}} = k \frac{V}{v_0} C_{A,0} + 1$$

$$\therefore C_{A,f} = \frac{C_{A,0}}{k \frac{V}{v_0} C_{A,0} + 1}$$

Entering the numerical values, we ultimately obtain

$$C_{A,f} = \frac{1.0}{1 + \frac{(0.05 \times 60) \times 1.0 \times 2.0}{0.5}} = \boxed{0.0769 \text{ mol/L}}$$

Factor 60 was added to change the dimensions of k from liter/mol·sec to liter/mol·min.

◆ The correct answer is **B**.

P.9 → Solution

For the reaction in question, equation (21) of Table 2 holds,

$$k \frac{C_{A,0} V}{F_{A,0}} = (1 + \varepsilon_A) \ln \left(\frac{1}{1 - X_A} \right) - \varepsilon_A X_A \quad (\text{I})$$

We must first evaluate the initial concentration of phosphine,

$$C_{A,0} = \frac{P_{A,0}}{RT} = \frac{2/3 \times 11.4}{0.0821 \times (649 + 273)} = 0.101 \text{ mol/L}$$

To determine the expansion factor, consider the following volume balance.

	4A → 7R
Reactants	40 → 70
Inerts	20 → 20

Accordingly,

$$\varepsilon_A = \frac{90 - 60}{60} = 0.5$$

We can now rearrange equation (I) and substitute our data, giving

$$V = \frac{F_{A,0}}{k C_{A,0}} \left[(1 + \varepsilon_A) \ln \left(\frac{1}{1 - X_A} \right) - \varepsilon_A X_A \right]$$

$$\therefore V = \frac{10}{10 \times 0.101} \times \left[(1 + 0.5) \times \ln \left(\frac{1}{1 - 0.75} \right) - 0.5 \times 0.75 \right] = \boxed{16.9 \text{ L}}$$

◆ The correct answer is **A**.

P.10 → Solution

For a second order reaction with expansion, the appropriate performance equation is equation (23) in Table 2,

$$V = \frac{v}{C_{A,0} k} \left[2\varepsilon_A (1 + \varepsilon_A) \ln(1 - X_A) + \varepsilon_A^2 X_A + (\varepsilon_A + 1)^2 \frac{X_A}{1 - X_A} \right]$$

The initial concentration of ozone (A) is given by the ideal gas law,

$$C_{A,0} = \frac{P_{A,0}}{RT} = \frac{0.2 \times 1.5}{0.0821 \times (273 + 93)} = 0.00998 \text{ mol/L}$$

The expansion factor is $\varepsilon_A = (11 - 10)/10 = 0.1$. Substituting these and other data in the equation for V , we get

$$V = \frac{1.0}{0.00998 \times 0.05} \times \left[2 \times 0.1 \times (1 + 0.1) \ln(1 - 0.5) + 0.1^2 \times 0.5 + (0.1 + 1)^2 \times \frac{0.5}{1 - 0.5} \right]$$

$$\therefore \boxed{V = 2130 \text{ L}}$$

◆ The correct answer is **C**.

P.11 → Solution

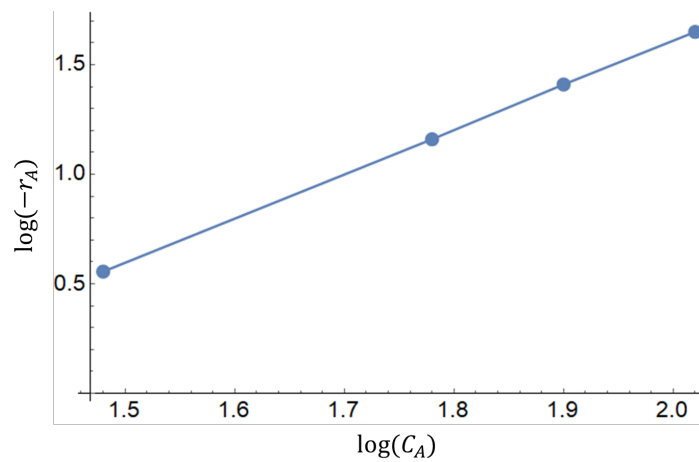
The rate $-r_A$ is given by

$$-r_A = \frac{C_{A,0} X_A v_0}{V} = \frac{C_{A,0} (C_{A,0} - C_A) v_0}{(C_{A,0} + \varepsilon_A C_A) V} = \frac{120(120 - C_A) v_0}{(120 + 2C_A) \times 1.0} \quad (\text{I})$$

where we have substituted $C_{A,0} = 120$ mmol/liter, $V = 1$ liter, and $\varepsilon_A = (3 - 1)/1 = 2.0$. The data are processed in the following table.

v_0 (L/min)	C_A (mmol/L)	$-r_A$ (Eq. I)	$\log(-r_A)$	$\log C_A$
0.06	30	3.6	0.556	1.48
0.48	60	14.4	1.16	1.78
1.5	80	25.7	1.41	1.90
8.1	105	44.2	1.65	2.02

The next step is to plot $\log(-r_A)$ (the blue column) versus $\log C_A$ (the red column), as follows.



The line is described by the relation

$$\log(-r_A) = \log k + n \log C_A$$

where n is the slope of the line (and the reaction order), which can be easily seen to be $n = 2.0$. Thus,

$$\log(-r_A) = \log k + 2.0 \log C_A$$

Substituting any of the data points available, we can determine rate constant k ,

$$0.556 = \log k + 2.0 \times 1.48$$

$$\therefore \log k = -2.40$$

$$\therefore k = 10^{-2.4} = 0.004$$

The appropriate expression for the reaction rate is

$$-r_A = k C_A^n = \boxed{0.004 C_A^2 \text{ mmol/lit} \cdot \text{min}}$$

♦ The correct answer is **D**.

P.12 → Solution

To begin, we write an expression for conversion X_A , as follows.

$$C_A = C_{A,0} (1 - X_A) \rightarrow X_A = 1 - \frac{C_A}{C_{A,0}}$$

$$\therefore X_A = 1 - \frac{C_A}{100} \quad (\text{I})$$

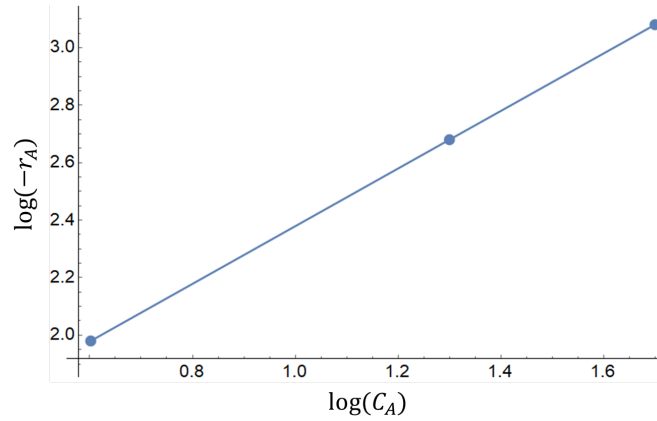
The reaction rate, in turn, is given by

$$-r_A = \frac{v_0 C_{A,0} X_A}{V} = \frac{v_0 \times 100 \times X_A}{1.0} = 100 v_0 X_A \quad (\text{II})$$

In order to establish the reaction order, we must plot $\log -r_A$ versus $\log C_A$. The data are processed in the following table.

v_0 (L/min)	C_A (mmol/L)	X_A (Eq. I)	$-r_A$ (Eq. II)	$\log(-r_A)$	$\log C_A$
1	4	0.96	96	1.98	0.602
6	20	0.8	480	2.68	1.30
24	50	0.5	1200	3.08	1.70

The graph we are looking for is one $\log(-r_A)$ (the blue column) versus $\log C_A$ (the red column), as follows.



The slope of the line is approximately 1. Thus, the reaction in question is a first-order reaction. It remains to compute the rate constant k , which is given by

$$-r_A = kC_A \rightarrow k = \frac{-r_A}{C_A}$$

Substituting one of the available data points, we obtain

$$k = \frac{96}{4} = 24 \text{ min}^{-1}$$

Thus, the rate equation is established as

$$-r_A = 24C_A \frac{\text{mmol}}{\text{liter} \cdot \text{min}}$$

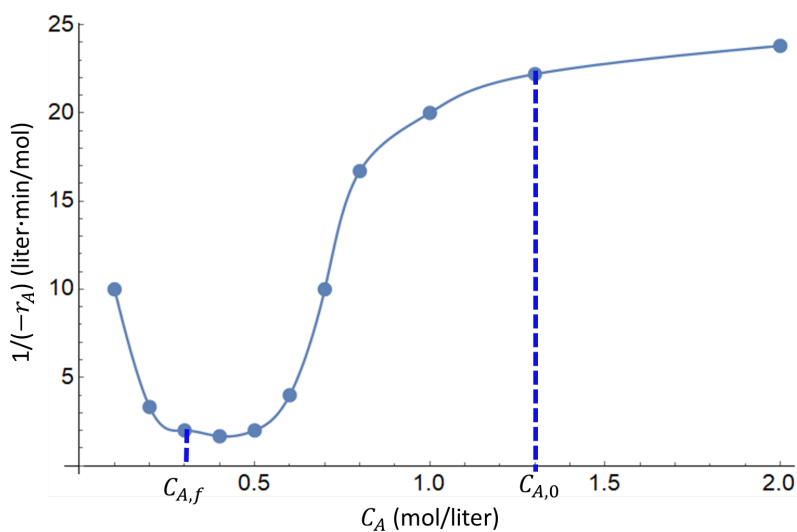
◆ The correct answer is **B**.

P.13 → Solution

Part 1: To begin, we tabulate values of $1/(-r_A)$.

C_A (mol/liter)	$-r_A$ (mol/liter·min)	$1/(-r_A)$
0.1	0.1	10
0.2	0.3	3.33
0.3	0.5	2
0.4	0.6	1.67
0.5	0.5	2
0.6	0.25	4
0.7	0.10	10
0.8	0.06	16.7
1.0	0.05	20
1.3	0.045	22.2
2.0	0.042	23.8

Then, a rate-concentration plot of $1/(-r_A)$ (the blue column) versus C_A (the red column) is prepared.



It can be easily seen that the time required to produce the concentration drop in question is given by

$$t = \int_{C_{A,f}}^{C_{A,0}} \frac{dC_A}{-r_A}$$

The result in the right-hand side is the area below the graph between abscissae $C_{A,f} = 0.3$ mol/L and $C_{A,0} = 1.3$ mol/L, which, using numerical integration, is found to equal 12.7 min. Accordingly,

$$t = \int_{C_{A,f}}^{C_{A,0}} \frac{dC_A}{-r_A} \approx \boxed{12.7 \text{ min}}$$

Note

In Mathematica, a quick way to go is to combine the *Integrate* and *Interpolation* commands. We first type the data,

```
dataSet = {{0.1,10}, {0.2,3.33}, {0.3,2}, {0.4,1.67}, {0.5,2}, {0.6,4}, {0.7,10},
           {0.8,16.7}, {1.,20}, {1.3,22.2}, {2.,23.8}}
```

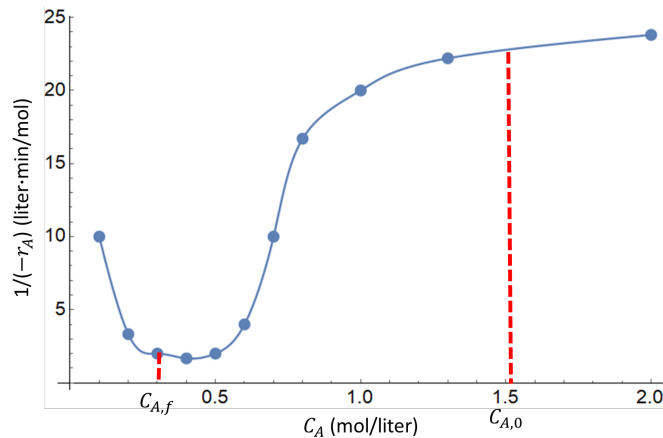
Then, we type

```
Integrate[Interpolation[dataSet][x], {x, 0.3,1.3}]
```

This returns 12.6978.

◆ The correct answer is **B**.

Part 2: The rate-concentration curve is replotted below.



The final concentration is, in this case,

$$C_A = C_{A,0}(1 - X_A) = 1.5 \times (1 - 0.8) = 0.3 \text{ mol/L}$$

For a plug flow reactor of constant density, we write

$$\tau = C_{A,0} \int_0^{X_{A,f}} \frac{dX_A}{-r_A} = - \int_{C_{A,0}}^{C_{A,f}} \frac{dC_A}{-r_A}$$

However, the space time $\tau = C_{A,0}V/F_{A,0}$, so that

$$\tau = \frac{C_{A,0}V}{F_{A,0}} = - \int_{C_{A,0}}^{C_{A,f}} \frac{dC_A}{-r_A} \rightarrow V = \frac{F_{A,0}}{C_{A,0}} \left[- \int_{1.5}^{0.3} \frac{dC_A}{-r_A} \right]$$

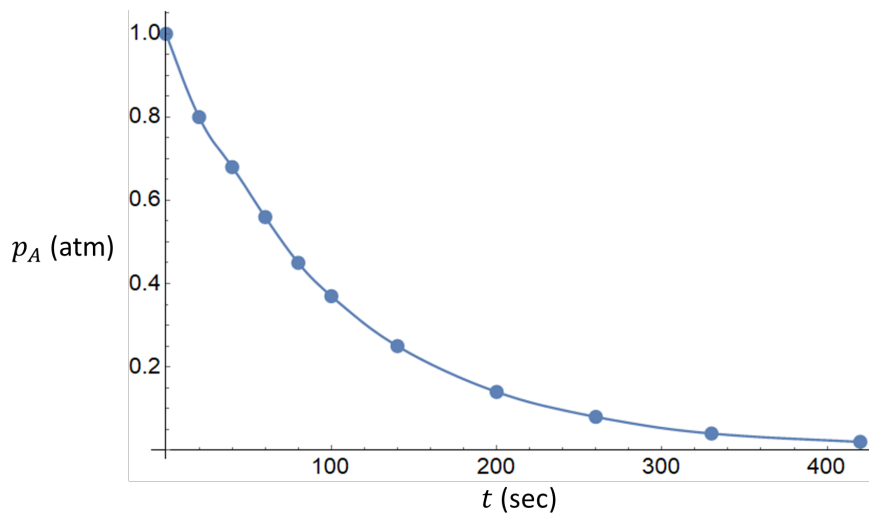
The integral in brackets equals the area below the rate-concentration curve between abscissae $C_{A,0} = 1.5$ mol/L and $C_{A,f} = 0.3$ mol/L. Using numerical integration, the result is found to be 17.2 min. Accordingly, the reactor volume becomes

$$V = \frac{(1000/60)}{1.5} \times 17.2 = \boxed{191 \text{ L}}$$

◆ The correct answer is **C**.

P.14 → **Solution**

Since there are 20% inerts in the feed, $p_{A,0} = 0.8 \times 1.0 = 0.8$ atm. For 95% conversion, the pressure at the outlet must be $p_{A,f} = 0.05 \times 0.8 = 0.04$ atm. For mixed flow, we must first find the rate at the exit conditions. Then we can proceed to determine the reactor size. Accordingly, we draw a p_A versus t curve and find the slope (and hence the rate) at $p_A = 0.04$ atm.



The slope at $p_A = 0.04$ atm can be approximated as

$$\text{rate} = \frac{0.02 - 0.08}{420 - 260} = -\frac{0.06}{160} \text{ atm/s}$$

The space time, written in pressure units, follows as

$$\tau = \frac{p_{A,0} - p_A}{-r_A} = \frac{0.8 - 0.04}{(0.06/160)} = 2030 \text{ s}$$

The molar feed, taking the flow of inerts into account, is $n_{\text{feed}} = 100 \times 100/80 = 125$ mol/hr. The volumetric flow rate can be obtained from the ideal gas law,

$$v = \frac{n_{\text{feed}} RT}{p} = \frac{125 \times 0.0821 \times 373}{1.0} = 3830 \text{ L/hr}$$

Finally, the reactor volume is calculated to be

$$V = \tau v = 2030 \times \left(3830 \times \frac{1}{3600} \right) = \boxed{2160 \text{ L}}$$

◆ The correct answer is **D**.

➤ ANSWER SUMMARY

Problem 1		T/F
Problem 2		B
Problem 3		D
Problem 4		A
Problem 5		D
Problem 6		C
Problem 7		C
Problem 8		B
Problem 9		A
Problem 10		C
Problem 11		D
Problem 12		B
Problem 13	13.1	B
	13.2	C
Problem 14		D

➤ REFERENCES

- FOGLER, H. (2018). *Essentials of Chemical Reaction Engineering*. 2nd edition. Upper Saddle River: Pearson.
- LEVENSPIEL, O. (1999). *Chemical Reaction Engineering*. 3rd edition. Hoboken: John Wiley and Sons.



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answer your question as soon as possible.