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## QUIZ CE201

## Ideal Reactors - Part 1

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## PROBLEMS

$>$ Problem 1 (Modified from Hill \& Root, 2014, w/ permission)
Inukai and Kojima studied the aluminum chloride-catalyzed diene condensation of butadiene and methyl acrylate in benzene solution. The stoichiometry for this Diels-Alder reaction is


The following set of mechanistic reactions is consistent with their experimental results.

$$
\begin{gathered}
\mathrm{AlCl}_{3}+\mathrm{M} \rightarrow \mathrm{AlCl}_{3} \cdot \mathrm{M} \text { (Fast) (A) } \\
\mathrm{B}+\mathrm{AlCl}_{3} \cdot \mathrm{M} \xrightarrow{k_{2}} \mathrm{C} \cdot \mathrm{AlCl}_{3} \text { (Slow) (B) } \\
\mathrm{C} \cdot \mathrm{AlCl}_{3} \rightarrow \mathrm{C}+\mathrm{AlCl}_{3} \text { (Fast) (C) }
\end{gathered}
$$

where reaction $(\mathrm{B})$ is the rate-limiting step. $\mathrm{AlCl}_{3} \cdot \mathrm{M}$ and $\mathrm{C} \cdot \mathrm{AlCl}_{3}$ represent complexes formed between the dissolved $\mathrm{AlCl}_{3}$ and the species in question. The concentration of the first reactive complex is essentially constant as long as enough methyl acrylate remains in solution to regenerate $\mathrm{AlCl}_{3} \cdot \mathrm{M}$ efficiently. The concentration of methyl acrylate in excess of $\mathrm{AlCl}_{3}$ will not affect the rate of reaction during the early stages of reaction, but as reaction proceeds and the methyl acrylate concentration drops below the initial $\mathrm{AlCl}_{3}$ concentration, the amount of complex present is limited by the amount of methyl acrylate remaining.

These investigators report that the second-order rate constant for reaction $B$ is equal to $1.21 \times 10^{-3} \mathrm{~m}^{3} /(\mathrm{mol} \cdot \mathrm{ks})$ at $20^{\circ} \mathrm{C}$. Determine the volume of plug flow reactor that would be necessary to achieve $50 \%$ conversion of the liquid butadiene assuming isothermal operating conditions and a liquid feed rate of $0.61 \mathrm{~m}^{3} / \mathrm{ks}$. The feed concentrations (in $\mathrm{mol} / \mathrm{m}^{3}$ ) are 96.5 for butadiene (B), 184 for methyl acrylate (M), and 7 for $\mathrm{AlCl}_{3}$.
A) $V=18.6 \mathrm{~m}^{3}$
B) $V=24.5 \mathrm{~m}^{3}$
C) $V=33.1 \mathrm{~m}^{3}$
D) $V=49.9 \mathrm{~m}^{3}$
$\rightarrow$ Problem 2 (Modified from Hill \& Root, 2014, w/ permission)
The Diels-Alder reaction of benzoquinone $(B)$ and cyclopentadiene $(C)$ is


$$
C+B \rightarrow \text { adduct } ; r=k C_{B} C_{C}
$$

Volume changes on reaction may be neglected. At $25^{\circ} \mathrm{C}$ the rate constant is equal to $0.01 \mathrm{~m}^{3} /(\mathrm{kmol} \cdot \mathrm{s})$. If one employs a well-stirred isothermal batch reactor to carry out this reaction, determine the holding time necessary to achieve 95\% conversion of the limiting agent using initial concentrations of 0.14 and 0.09 $\mathrm{kmol} / \mathrm{m}^{3}$ for cyclopentadiene and benzoquinone, respectively.
A) $t=0.522 \mathrm{~h}$
B) $t=0.814 \mathrm{~h}$
C) $t=1.14 \mathrm{~h}$
D) $t=1.56 \mathrm{~h}$

## $>$ Problem 3 (Modified from Schmal, 2014, w/ permission)

The reaction $A \rightarrow R+S$ is irreversible and first order. It is conducted in a PFR with 80 tubes, each with diameter of 5 cm and height of $1 \mathrm{~m} .200 \mathrm{~kg} / \mathrm{h}$ of reactant $A(M W=60 \mathrm{~g} / \mathrm{mol})$ with $30 \%$ inerts is introduced at a pressure of 50 bar and $600^{\circ} \mathrm{C}$. The output conversion is $90 \%$. Calculate the average residence time.
A) $\bar{t}=1.02 \mathrm{~min}$
B) $\bar{t}=1.93 \mathrm{~min}$
C) $\bar{t}=2.88 \mathrm{~min}$
D) $\bar{t}=3.56 \mathrm{~min}$

## $>$ Problem 4 (Modified from Schmal, 2014, w/ permission)

A gas phase reaction $A+B \rightarrow R$ is carried out in a CSTR and PFR separately at a rate of $120 \mathrm{~mol} / \mathrm{min}$ where the temperature is constant at $150^{\circ} \mathrm{C}$ and the pressure is 10.8 atm. The reactant $B$ is three times greater than $A$ in the feed reactor. The rate constant is given by $\ln k=-5550 / T+12.5 \mathrm{~min}^{-1}$, with $T$ in K. If the average residence time in the PFR is 2.5 min and assuming equal values of conversion on outputs of each reactor, find the volumes of each reactor and determine the ratio $V_{C S T R} / V_{P F R}$.
A) $V_{C S T R} / V_{P F R}=1.04$
B) $V_{C S T R} / V_{P F R}=1.39$
C) $V_{C S T R} / V_{P F R}=1.71$
D) $V_{C S T R} / V_{P F R}=2.01$

## Problem 5 (Modified from Schmal, 2014, w/ permission)

A second-order irreversible reaction $A \rightarrow 2 R$ is carried out in gas phase in a PFR reactor. A reactant ( $M W=40$ ) with $50 \%$ by weight and the rest with an inert $\left(M W_{\text {inert }}=20\right)$ are introduced into the PFR. The reaction is conducted at a pressure of 5.25 atm and a temperature of $70^{\circ} \mathrm{C}$, which is kept constant in the process. The rate constant is $400 \mathrm{~m}^{3} /(\mathrm{kmol} \cdot \mathrm{ks})$. Suppose we wish to produce $30 \mathrm{kmol} / \mathrm{h}$ of product $R$, knowing that the final conversion was $40 \%$. Calculate the volume of the reactor.
A) $V=2.44 \mathrm{~m}^{3}$
B) $V=4.82 \mathrm{~m}^{3}$
C) $V=6.91 \mathrm{~m}^{3}$
D) $V=8.50 \mathrm{~m}^{3}$

## Problem 6 (Modified from Ravi et al., 2014, w/ permission)

Styrene is to be produced by the catalytic dehydrogenation of ethylbenzene according to the reaction

$$
\mathrm{C}_{6} \mathrm{H}_{5} \cdot \mathrm{CH}_{2} \cdot \mathrm{CH}_{3} \rightleftharpoons \mathrm{C}_{6} \mathrm{H}_{5} \cdot \mathrm{CH}: \mathrm{CH}_{2}+\mathrm{H}_{2}
$$

The rate equation for this reaction takes the form

$$
r=k\left(P_{\mathrm{Et}}-\frac{1}{K_{p}} P_{\mathrm{St}} P_{H}\right)
$$

where $P_{\mathrm{Et}}, P_{\mathrm{St}}$, and $P_{H}$ are the partial pressures of ethylbenzene, styrene, and hydrogen, respectively. The reactor will consist of a number of tubes each of 80 mm diameter packed with catalyst with a bulk density of $1440 \mathrm{~kg} / \mathrm{m}^{3}$. The ethylbenzene will be diluted with steam, the feed rates being $1.6 \times 10^{-3} \mathrm{kmol} / \mathrm{m}^{2} \mathrm{~s}$ for
ethylbenzene and $29 \times 10^{-3} \mathrm{kmol} / \mathrm{m}^{2} \mathrm{~s}$ for steam. The reactor will be operated at a mean pressure of $120 \mathrm{kN} / \mathrm{m}^{2}$ (1.2 bar) and the temperature will be maintained at $833 \mathrm{~K}\left(560^{\circ} \mathrm{C}\right)$ throughout. If the fractional conversion of benzene is to be 0.45 , estimate the length and number of tubes required to produce $0.231 \mathrm{~kg} / \mathrm{s}(=20$ tonne/day) of styrene. At $833 \mathrm{~K}, k=6.6 \times 10^{-6} \mathrm{kmol} /\left(\mathrm{kg}\right.$ catalyst-bar-sec) and $K_{p}=$ $1.0 \times 10^{4} \mathrm{~N} / \mathrm{m}^{2}$.
A) $L=1.77 \mathrm{~m}$ and number of tubes $=308$
B) $L=1.77 \mathrm{~m}$ and number of tubes $=615$
C) $L=3.54 \mathrm{~m}$ and number of tubes $=308$
D) $L=3.54 \mathrm{~m}$ and number of tubes $=615$

## $>$ Problem 7 (Modified from Ravi et al., 2014, w/ permission)

A substance $A$ reacts with a second substance $B$ to give a desired product $P$, but $B$ also undergoes a simultaneous side reaction to give an unwanted product $Q$ as follows.

$$
\begin{aligned}
\mathrm{A}+\mathrm{B} & \rightarrow \mathrm{P} ; \text { Rate }=k_{P} C_{A} C_{B} \\
2 \mathrm{~B} & \rightarrow \mathrm{Q} ; \text { Rate }=k_{Q} C_{B}^{2}
\end{aligned}
$$

where $C_{A}$ and $C_{B}$ are the concentrations of A and B , respectively. A single continuous stirred tank reactor is used for these reactions. $A$ and $B$ are mixed in equimolar proportions such that each has the concentration $C_{0}$ in the combined stream fed at a volumetric flow rate $v$ to the reactor. If the rate constants above are $k_{P}=k_{Q}=k$ and the total conversion of $B$ is 0.95 , that is, the concentration of $B$ in the outflow is $0.05 C_{0}$, determine the volume of the reactor and the relative yield of $P$.
A) Reactor volume $=35.3 v / k C_{0}$ and $\phi=0.455$
B) Reactor volume $=35.3 v / k C_{0}$ and $\phi=0.814$
C) Reactor volume $=70.6 v / k C_{0}$ and $\phi=0.455$
D) Reactor volume $=70.6 v / k C_{0}$ and $\phi=0.814$

## Problem 8 (Modified from Ravi et al., 2014, w/ permission)

Two stirred tanks are available, one $100 \mathrm{~m}^{3}$ in volume, the other $30 \mathrm{~m}^{3}$ in volume. It is suggested that these tanks be used as a two-stage CSTR for carrying out a liquid phase reaction $A+B \rightarrow$ Product. The two reactants will be present in the feed stream in equimolar proportions, the concentration of each being $1.5 \mathrm{kmol} / \mathrm{m}^{3}$. The volumetric flow rate of the feed stream will be $0.3 \times 10^{-3} \mathrm{~m}^{3} / \mathrm{s}$. The reaction is irreversible and is of first order with respect to each of the reactants $A$ and $B$, i.e. second order overall, with a rate constant $1.8 \times 10^{-4} \mathrm{~m}^{3} / \mathrm{kmol} \cdot \mathrm{s}$. Which tank should be used as the first stage of the reactor system, the aim being to effect as high an overall conversion as possible?

## $>$ Problem 9 (Modified from Hill \& Root, 2014, w/ permission)

Reconsider the Diels-Alder reaction between benzoquinone (B) and cyclopentadiene (C) discussed in Problem 2, namely

$$
\mathrm{B}+\mathrm{C} \rightarrow \text { Adduct }
$$

If one employs a feed containing equimolal concentrations of reactants, the reaction rate expression can be written as

$$
r=k C_{C} C_{B}=k C_{B}^{2}
$$

Determine the reactor size requirements for cascades composed of one, two, and three identical CSTRs. Use an algebraic approach and assume isothermal operation at $25^{\circ} \mathrm{C}$ where the reaction rate constant is equal to $10.4 \mathrm{~m}^{3} /(\mathrm{kmol} \cdot \mathrm{ks})$. Reactant concentrations in the feed are equal to $0.075 \mathrm{kmol} / \mathrm{m}^{3}$. The liquid feed rate is equal to $0.28 \mathrm{~m}^{3} / \mathrm{ks}$. The desired degree of conversion is equal to $90 \%$.

| 1. Individual reactor <br> volume for one CSTR | A) $54.1 \mathrm{~m}^{3}$ B) $44.5 \mathrm{~m}^{3}$ C) $32.2 \mathrm{~m}^{3}$ D) $20.5 \mathrm{~m}^{3}$ |
| :---: | :---: |
| 2. Individual reactor <br> volume for a cascade <br> of two CSTRs | A) $14.4 \mathrm{~m}^{3}$ B) $10.2 \mathrm{~m}^{3}$ C) $7.14 \mathrm{~m}^{3}$ D) $4.88 \mathrm{~m}^{3}$ |
| 3. Individual reactor <br> volume for a cascade <br> of three CSTRs | A) $4.28 \mathrm{~m}^{3}$ B) $2.24 \mathrm{~m}^{3}$ C) $0.911 \mathrm{~m}^{3}$ D) $0.347 \mathrm{~m}^{3}$ |

## - Problem 10 (Fogler, 2018, w/ permission)

The adiabatic exothermic irreversible gas-phase reaction

$$
2 \mathrm{~A}+\mathrm{B} \rightarrow 2 \mathrm{C}
$$

is to be carried out in a flow reactor for an equimolar feed of A and B. A Levenspiel plot for this reaction is shown below. True or false?

1.( ) The PFR volume required to achieve $50 \%$ conversion is greater than $120,000 \mathrm{~m}^{3}$. 2. ( ) The CSTR volume required to achieve $50 \%$ conversion is greater than $60,000 \mathrm{~m}^{3}$. 3.( ) Suppose we added a second CSTR to the CSTR introduced in statement 2. For an overall conversion of $80 \%$, the second CSTR must have a volume greater than 140,000 m³.
4. ( ) Suppose we added a PFR to the CSTR introduced in statement 2. For an overall conversion of $80 \%$, the PFR must have a volume greater than $100,000 \mathrm{~m}^{3}$.

## Problem 11 (Fogler, 2018, w/ permission)

The exothermic reaction of stilbene $(A)$ to form the economically important troposphene $(B)$ and methane $(C)$ follows the reaction

$$
\mathrm{A} \rightarrow \mathrm{~B}+\mathrm{C}
$$

The following data was recorded. The entering molar flow rate of A was $300 \mathrm{~mol} / \mathrm{min}$. True or false?

| $X$ | 0 | 0.2 | 0.4 | 0.45 | 0.5 | 0.6 | 0.8 | 0.9 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $-r_{A}\left(\mathrm{~mol} / \mathrm{dm}^{3} \cdot \mathrm{~min}\right)$ | 1.0 | 1.67 | 5.0 | 5.0 | 5.0 | 5.0 | 1.25 | 0.91 |

1.( ) The PFR volume required to achieve $40 \%$ conversion is greater than $60 \mathrm{dm}^{3}$.
2.( ) The CSTR volume required to achieve $40 \%$ conversion is greater than $30 \mathrm{dm}^{3}$.
3.( ) The conversion achieved by a $72-\mathrm{dm}^{3}$ PFR followed in series by a $24-\mathrm{dm}^{3}$ CSTR is greater than 0.75 .
4.( ) The conversion achieved by a $24-\mathrm{dm}^{3}$ CSTR followed in series by a $72-\mathrm{dm}^{3}$ PFR is greater than 0.8.

## SOLUTIONS

## P. $1 \rightarrow$ Solution

Butadiene is the limiting agent and conversions will be expressed in terms of this species. Over the composition range of interest, sufficient methyl acrylate will always be present to tie up the aluminum chloride as the complex $\mathrm{AlCl}_{3} \cdot \mathrm{M}$. Consequently, the concentration of the complex $\mathrm{AlCl}_{3} \cdot \mathrm{M}$ will remain constant throughout the length of the reactor at a value equal to the initial $\mathrm{AlCl}_{3}$ concentration. For these conditions the reaction rate takes the form

$$
-r_{B}=k C_{B} C_{\mathrm{AlCl}_{3} \cdot \mathrm{M}}=k C_{B, 0}\left(1-X_{B}\right) C_{\mathrm{AlCl}_{3}, 0}
$$

because the volume change accompanying liquid-phase reactions is negligible. The basic design relation is

$$
\tau=C_{B, 0} \int_{0}^{X_{B}} \frac{d X_{B}}{-r_{B}}=C_{B, 0} \int_{0}^{X_{B}} \frac{d X_{B}}{k C_{B, 0}\left(1-X_{B}\right) C_{\mathrm{AlCl}_{3}, 0}}
$$

Since $C_{A l C l_{3}, 0}$ and $k$ are constant for the conditions cited, the equation above can be integrated to give

$$
\begin{gathered}
\tau=\int_{0}^{X_{B}} \frac{d X_{B}}{k \rightarrow\left(1-X_{B}\right) C_{\mathrm{AlCl}_{3}, 0}}=\frac{1}{k C_{\mathrm{AlCl}_{3}, 0}} \int_{0}^{X_{B}} \frac{d X_{B}}{1-X_{B}} \\
\therefore \tau=\frac{1}{k C_{\mathrm{AlCl}_{3}, 0}} \times\left.\left[-\ln \left(1-X_{B}\right)\right]\right|_{0} ^{X_{B}} \\
\therefore \tau=-\frac{1}{k C_{A l C l_{3}, 0}} \ln \left(1-X_{B}\right)
\end{gathered}
$$

Substituting the pertaining variables brings to

$$
\tau=-\frac{1}{k C_{\mathrm{AlCl}_{3}, 0}} \ln \left(1-X_{B}\right)=-\frac{1}{\left(1.21 \times 10^{-3}\right) \times 7.0} \times \ln (1-0.5)=81.8 \mathrm{ks}=22.7 \mathrm{~h}
$$

Given $v_{0}=0.61 \mathrm{~m}^{3} / \mathrm{ks}$ and using the definition of space time, we write

$$
\begin{gathered}
\tau=\frac{V}{v_{0}} \rightarrow V=\tau v_{0} \\
\therefore V=81.8 \times 0.61=49.9 \mathrm{~m}^{3}
\end{gathered}
$$

- The correct answer is D.


## P. $2 \rightarrow$ Solution

The general form of the design equation for a batch reactor is

$$
t_{2}-t_{1}=N_{A, 0} \int_{X_{A, 1}}^{X_{A, 2}} \frac{d X_{A}}{\left(-r_{A}\right) V}
$$

where $N_{A, 0}$ is the number of moles of reactant A present when the fraction conversion is zero, and $V$ is the volume occupied by the reacting fluid. If time $t_{1}=0$ and conversion $X_{A, 1}=0$, the equation simplifies to

$$
t=N_{A, 0} \int_{0}^{X_{A}} \frac{d X_{A}}{\left(-r_{A}\right) V}
$$

The equation simplifies further if the reactor volume (fluid density) is constant, giving

$$
t=C_{A, 0} \int_{0}^{f_{A}} \frac{d X_{A}}{\left(-r_{A}\right)}=-\int_{C_{A, 0}}^{C_{A}} \frac{d C_{A}}{\left(-r_{A}\right)}
$$

This is the form of the equation applicable to the present problem. The rate of disappearance of benzoquinone (the limiting species) is written in terms of the initial concentrations and the fraction conversion as

$$
-r_{B}=k\left[C_{B, 0}\left(1-X_{B}\right)\right]\left(C_{C, 0}-X_{B} C_{B, 0}\right)
$$

so that

$$
t=C_{B, 0} \int_{0}^{X_{B}} \frac{d X_{B}}{k C_{B, 0}\left(1-X_{B}\right)\left(C_{C, 0}-X_{B} C_{B, 0}\right)}
$$

Integrating and simplifying, we get

$$
t=\frac{\ln \left[\frac{\left(\frac{C_{C, 0}}{C_{B, 0}}-X_{B}\right) \frac{C_{B, 0}}{C_{C, 0}}}{1-X_{B}}\right]}{k\left(C_{C, 0}-C_{B, 0}\right)}
$$

Substituting each variable brings to

$$
t=\frac{\ln \left[\frac{\left(\frac{0.14}{0.09}-0.95\right) \times \frac{0.09}{0.14}}{1-0.95}\right]}{0.01 \times(0.14-0.09)}=4100 \mathrm{~s}=1.14 \mathrm{~h}
$$

The holding time necessary for the desired conversion level is about one hour and eight minutes.

- The correct answer is C.


## P. $3 \rightarrow$ Solution

For a first-order reaction in a PFR, the space time is given by

$$
\tau=-\frac{1}{k}\left[\left(1+\varepsilon_{A}\right) \ln \left(1-X_{A}\right)+\varepsilon_{A} X_{A}\right](\mathrm{I})
$$

The mass flow in each tube is $\grave{m}=200 / 80=1.25 \mathrm{~kg} / \mathrm{h}$. In a molar basis, we have $F_{A, 0}=1.25 / 60=0.0208 \mathrm{kmol} / \mathrm{h}=20.8 \mathrm{~mol} / \mathrm{h}$. The initial concentration of A is

$$
C_{A, 0}=\frac{p_{A, 0}}{R T}=\frac{0.7 \times 50}{0.0821 \times 873}=0.488 \mathrm{~mol} / \mathrm{L}
$$

Since $F_{A, 0}=C_{A, 0} v_{0}$, the initial volumetric flow is found as

$$
\begin{gathered}
F_{A, 0}=C_{A, 0} v_{0} \rightarrow v_{0}=\frac{F_{A, 0}}{C_{A, 0}} \\
\therefore v_{0}=\frac{20.8}{0.488}=42.6 \mathrm{~L} / \mathrm{h}=0.71 \mathrm{~L} / \mathrm{min}
\end{gathered}
$$

The volume of an individual tube is

$$
V=\frac{\pi d^{2}}{4} \times \ell=\frac{\pi \times 5^{2}}{4} \times 100=1960 \mathrm{~cm}^{3}=1.96 \mathrm{~L}
$$

so that

$$
\begin{gathered}
V=\tau v_{0} \rightarrow \tau=\frac{V}{v_{0}} \\
\therefore \tau=\frac{1.96}{0.71}=2.76 \mathrm{~min}
\end{gathered}
$$

Expansion parameter $\varepsilon_{A}$ is determined next.

|  | A | R | S | Inert | Total |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Initial | 0.7 | 0 | 0 | 0.3 | 1.0 |
| Final | 0 | 0.7 | 0.7 | 0.3 | 1.7 |

Accordingly, $\varepsilon_{A}=(1.7-1.0) / 1.0=0.7$. We can now substitute our data in equation (I) and establish the rate constant $k$,

$$
\begin{gathered}
2.76=-\frac{1}{k} \times[(1+0.7) \ln (1-0.9)+0.7 \times 0.9] \\
\therefore 2.76=-\frac{1}{k} \times(-3.28) \\
\therefore k=\frac{3.28}{2.76}=1.19 \mathrm{~min}^{-1}
\end{gathered}
$$

Lastly, the average residence time is given by

$$
\bar{t}=-\frac{1}{k} \ln \left(1-X_{A}\right)=-\frac{1}{1.19} \ln (1-0.9)=1.93 \mathrm{~min}
$$

- The correct answer is $\mathbf{B}$.


## P. $4 \rightarrow$ Solution

The ratio of reactants, $B / A=3$, indicates that there is a large dilution.
Therefore, A is limiting. Since $k$ is given in $\mathrm{min}^{-1}$, we can surmise that the reaction is first order, but with variable volume; that is,

$$
-r_{A}=k C_{A}=\frac{C_{A, 0}\left(1-X_{A}\right)}{1+\varepsilon_{A} X_{A}}
$$

The average residence time is then

$$
\bar{t}=C_{A, 0} \int_{0}^{X_{A}} \frac{d X_{A}}{\left(1+\varepsilon_{A} X_{A}\right)\left(-r_{A}\right)}
$$

Replacing $-r_{A}$ and carrying out the integration, we get

$$
\bar{t}=-\frac{1}{k} \ln \left(1-X_{A}\right)
$$

Given the reaction temperature $T=150+273=423 \mathrm{~K}$, the rate constant is determined as

$$
\begin{gathered}
\ln k=-\frac{5550}{T}+12.5=-\frac{5550}{423}+12.5=-0.621 \\
\therefore k=0.537 \mathrm{~min}^{-1}
\end{gathered}
$$

Since $\bar{t}=2.5 \mathrm{~min}$, it follows that

$$
2.5=-\frac{1}{0.537} \times \ln \left(1-X_{A}\right) \rightarrow X_{A}=0.739
$$

The performance equation for the PFR is

$$
\tau=\frac{V}{v_{0}}=C_{A, 0} \int_{0}^{X_{A}} \frac{d X_{A}}{-r_{A}}
$$

which, substituting $r_{A}$ and integrating, gives

$$
\tau=-\frac{1}{k}\left[\left(1+\varepsilon_{A}\right) \ln \left(1-X_{A}\right)+\varepsilon_{A} X_{A}\right]
$$

The expansion parameter is determined from the following volume balance.

|  | A | B | R | Total |
| :---: | :---: | :---: | :---: | :---: |
| Initial | 1 | 3 | 0 | 4 |
| Final | 0 | 2 | 1 | 3 |

Accordingly, $\varepsilon_{A}=(3-4) / 4=-0.25$. Substituting in the equation for $\tau$ brings to

$$
\tau=-\frac{1}{0.537} \times[(1-0.25) \ln (1-0.739)-0.25 \times 0.739]=2.22 \mathrm{~min}
$$

The initial molar flow of $A$ is determined as

$$
\begin{gathered}
F_{A, 0}+F_{B, 0}=120 \\
\therefore F_{A, 0}+3 F_{A, 0}=120 \\
\therefore F_{A, 0}=30 \mathrm{~mol} / \mathrm{min}
\end{gathered}
$$

The initial concentration is

$$
C_{0}=\frac{p}{R T}=\frac{10.8}{0.0821 \times 423}=0.311 \mathrm{~mol} / \mathrm{L}
$$

The initial volume flow rate is then

$$
v_{0}=\frac{F_{0}}{C_{0}}=\frac{120}{0.311}=386 \mathrm{~L} / \mathrm{min}
$$

Lastly, the volume of the PFR reactor is

$$
V_{\mathrm{PFR}}=v_{0} \tau=386 \times 2.22=857 \mathrm{~L}
$$

Consider now the volume of the CSTR reactor. The design equation is, in this case,

$$
\frac{V}{v_{0}}=\tau=C_{A, 0} \frac{X_{A}}{\left(-r_{A}\right)}
$$

Substituting the expression we have for $-r_{A}$ and other data, we get

$$
\begin{gathered}
\tau=C_{A, 0} \frac{X_{A}}{\left(-r_{A}\right)}=C_{A, 0} \frac{X_{A}}{\frac{C / A, 0}{1+\varepsilon_{A} X_{A}}}=\frac{X_{A}\left(1+\varepsilon_{A} X_{A}\right)}{1-X_{A}} \\
\therefore \tau=\frac{0.739 \times(1-0.25 \times 0.739)}{1-0.739}=2.31 \mathrm{~min}
\end{gathered}
$$

With the same input flow, we have

$$
V_{C S T R}=v_{0} \tau=386 \times 2.31=892 \mathrm{~L}
$$

Finally, the ratio of volumes is determined to be

$$
\frac{V_{C S T R}}{V_{P F R}}=\frac{892}{857}=1.04
$$

- The correct answer is $\mathbf{A}$.


## P. $5 \Rightarrow$ Solution

Since the reaction has second order kinetics, we can write

$$
-r_{A}=k C_{A}^{2}=\frac{k C_{A, 0}^{2}\left(1-X_{A}\right)^{2}}{\left(1+\varepsilon_{A} X_{A}\right)^{2}}
$$

Substituting in the PFR equation and integrating, we get

$$
\begin{gathered}
\tau=\frac{V}{v_{0}}=C_{A, 0} \int_{0}^{X_{A}} \frac{d X_{A}}{-r_{A}} \\
\therefore \tau=\frac{1}{k C_{A, 0}}\left[\left(1+\varepsilon_{A}\right)^{2} \frac{X_{A}}{1-X_{A}}+\varepsilon_{A}^{2} X_{A}+2 \varepsilon_{A}\left(1+\varepsilon_{A}\right) \ln \left(1-X_{A}\right)\right]
\end{gathered}
$$

To calculate $\varepsilon_{A}$, consider that, in a $1.0-\mathrm{g}$ sample of reagent mixture, we have $0.5 / 40=0.0125 \mathrm{~mol}$ of $A$ and $0.5 / 20=0.025 \mathrm{~mol}$ of inert. Then, the following volume balance is prepared.

|  | A | 2 R | Inert | Total |
| :---: | :---: | :---: | :---: | :---: |
| Initial | 0.0125 | 0 | 0.025 | 0.0375 |
| Final | 0 | 0.025 | 0.025 | 0.05 |

The expansion parameter is $\varepsilon_{A}=(0.05-0.0373) / 0.0373=0.340$. The initial concentration of $A$ is given by

$$
C_{A, 0}=\frac{y_{A, 0} p}{R T}=\frac{0.33 \times 5.25}{0.0821 \times 343}=0.0615 \mathrm{~mol} / \mathrm{L}
$$

or, equivalently, $C_{A, 0}=0.0615 \mathrm{kmol} / \mathrm{m}^{3}$. Substituting the pertinent quantities in equation (I), we obtain

$$
\begin{gathered}
\tau=\frac{1}{400 \times 0.0615} \times\left[(1+0.33)^{2} \times \frac{0.35}{1-0.35}+0.33^{2} \times 0.35+2 \times 0.33 \times(1+0.33) \ln (1-0.35)\right] \\
\therefore \tau=0.0249 \mathrm{ks}=24.9 \mathrm{~s}=0.00692 \mathrm{~h}
\end{gathered}
$$

Given the output molar flow $F_{R}=30 \mathrm{kmol} / \mathrm{h}$, we can easily determine volumetric flow $v_{0}$,

$$
\begin{gathered}
F_{R}=C_{R} v_{0}=2 C_{A, 0} v_{0} X_{A} \rightarrow v_{0}=\frac{F_{R}}{2 C_{A, 0} X_{A}} \\
\therefore v_{0}=\frac{30}{2 \times 0.0615 \times 0.35}=697 \mathrm{~m}^{3} / \mathrm{h}
\end{gathered}
$$

In view of the two preceding results, the reactor volume is

$$
V=\tau v_{0}=0.00692 \times 697=4.82 \mathrm{~m}^{3}
$$

- The correct answer is $\mathbf{B}$.


## P. $6 \Rightarrow$ Solution

The fraction conversion of ethylbenzene is 0.45 , with the result that 1 kmol of ethylbenzene feed produces 0.45 kmol of styrene. The molar mass of styrene is $104 \mathrm{~kg} / \mathrm{kmol}$. Thus, 1 kmol of ethylbenzene feed produces $0.45 \times 104=46.8 \mathrm{~kg}$ styrene. The feed rate of ethylbenzene is then $1 \times 0.231 / 46.8=0.00494 \mathrm{kmol} / \mathrm{s}$. The feed rate of ethylbenzene per unit cross-sectional area is $0.0016 \mathrm{kmol} / \mathrm{m}^{2} \mathrm{~s}$, and the cross-sectional area of all the tubes in the reactor is $A_{\text {Total }}=$ $0.00494 / 0.0016=3.09 \mathrm{~m}^{2}$. The cross-sectional area of a single tube is $A_{\text {Tube }}=\pi \times$ $0.08^{2} / 4=0.00503 \mathrm{~m}^{2}$. The number of tubes required follows as

$$
\text { Number of tubes required }=\left\lceil\frac{A_{\text {Total }}}{A_{\text {Tube }}}\right\rceil=\left\lceil\frac{3.09}{0.00503}\right\rceil=615
$$

In order to compute the length of the tubes, we require the mass $W$ of catalyst. This can be obtained with the tubular reactor design equation

$$
\frac{W}{F_{A}}=\int_{0}^{X_{f}} \frac{d X}{-r_{A}}
$$

The rate of reaction $r_{A}$ must be expressed in terms of the fractional conversion $X$. Considering 1 kmol of ethylbenzene entering the reactor at a total pressure of $P$ bar, the following mass balance is proposed. Bear in mind that the amount of steam produced in the reaction with 1 kmol of ethylbenzene is $1.0 \times$ $29 / 1.6=18.1 \mathrm{kmol}$.

|  | In <br> (kmol) | Out |  |  |
| :---: | :---: | :---: | :---: | :---: |
|  |  | (mole fraction) | (partial pressure) |  |
| Ethylbenzene | 1.0 | $1-X$ | $(1-$ <br> $X) /(19.1+X)$ | $(1-X) P /(19.1+X)$ |
| Styrene | - | $X$ | $X /(19.1+X)$ | $X P /(19.1+X)$ |
| Hydrogen | - | $X$ | $X /(19.1+X)$ | $X P /(19.1+X)$ |
| Steam | 18.1 | 18.1 | $18.1 /(19.1+X)$ | $18.1 P /(19.1+X)$ |
| Total | 19.1 | $19.1+X$ | 1 | $P$ |

Thus,

$$
-r_{A}=k\left[\frac{(1-X) P}{19.1+X}-\frac{X^{2}}{(19.1+X)^{2}} \frac{P^{2}}{K_{P}}\right]
$$

Substituting $P=1.2$ bar, $K_{p}=0.1$ bar and manipulating,

$$
\begin{gathered}
-r_{A}=k\left[\frac{(1-X) P}{19.1+X}-\frac{X^{2}}{(19.1+X)^{2}} \frac{P^{2}}{K_{P}}\right]=k\left[\frac{(1-X) \times 1.2}{19.1+X}-\frac{X^{2} \times 1.2^{2}}{(19.1+X)^{2} \times 0.1}\right] \\
\therefore-r_{A}=1.2 k\left[\frac{(1-X)}{19.1+X}-\frac{1.2 X^{2}}{(19.1+X)^{2} \times 0.1}\right] \\
\therefore-r_{A}=1.2 k\left[\frac{(1-X) \times(19.1+X) \times 0.1-1.2 X^{2}}{(19.1+X)^{2} \times 0.1}\right] \\
\therefore-r_{A}=1.2 k\left[\frac{19.1-18.1-13 X^{2}}{(19.1+X)^{2}}\right]
\end{gathered}
$$

Replacing $r_{A}$ in equation (I) brings to

$$
\frac{W}{F_{A}}=\frac{1}{1.2 k}\left[\int_{0}^{X_{F}} \frac{(19.1+X)^{2} d X}{19.1-18.1-13 X^{2}}\right]
$$

Evaluating the integral above with $X_{F}=0.45$ yields 12.6. Given $F_{A}=$
$0.00494 \mathrm{kmol} / \mathrm{s}$ and $k=6.6 \times 10^{-6} \mathrm{kmol} / \mathrm{kg}$ catalyst-bar-s, the mass of catalyst is found as

$$
\begin{gathered}
\frac{W}{F_{A}}=\frac{12.6}{1.2 k} \rightarrow W=\frac{12.6 F_{A}}{1.2 k} \\
\therefore W=\frac{12.6 \times 0.00494}{1.2 \times\left(6.6 \times 10^{-6}\right)}=7860 \mathrm{~kg}
\end{gathered}
$$

Since the catalyst has a density of $1440 \mathrm{~kg} / \mathrm{m}^{3}$, the volume of catalyst required is $V_{C}=7860 / 1440=5.46 \mathrm{~m}^{3}$. The volume of catalyst in each tube is $v_{C}=$ $5.46 / 615=0.00888 \mathrm{~m}^{3}$. Lastly, the length of each tube is calculated to be

$$
L=\frac{0.00888}{\left(\frac{\pi}{4} \times 0.08^{2}\right)}=1.77 \mathrm{~m}
$$

- The correct answer is $\mathbf{B}$.


## P. $7 \Rightarrow$ Solution

A material balance over the tank for material A at steady state gives

$$
\begin{gathered}
\text { In }- \text { Out }- \text { Reaction }=\text { Accumulation } \\
\therefore v C_{A, 0}-v C_{A}-k_{P} C_{A} C_{B} V=0
\end{gathered}
$$

The fractional conversion of $B$ is $\beta=0.95$. If the fractional conversion of $A$ is $\alpha$, noting that $\alpha<\beta$ since A is consumed in the first reaction only, whereas B is consumed in both, then

$$
\begin{aligned}
& C_{A}=C_{A, 0}(1-\alpha) \\
& C_{B}=C_{B, 0}(1-\beta) \\
& C_{A, 0}=C_{B, 0}=C_{0}
\end{aligned}
$$

Using these expressions, the material balance becomes

$$
\begin{gathered}
v C_{0}-v C_{0}(1-\alpha)-k_{P} V C_{0}^{2}(1-\alpha)(1-\beta)=0 \\
\therefore \alpha=\frac{k_{P} C_{0} V}{v}(1-\alpha)(1-\beta)
\end{gathered}
$$

In a similar manner, we apply a material balance for substance B,
In - Out - Reaction $=$ Accumulation

$$
\therefore v C_{B, 0}-v C_{B}-V\left(k_{P} C_{A} C_{B}+k_{Q} C_{B}^{2}\right)=0
$$

or

$$
\begin{gathered}
v C_{0}-v C_{0}(1-\beta)-V C_{0}^{2}\left[k_{P}(1-\alpha)(1-\beta)+k_{Q}(1-\beta)^{2}\right]=0 \\
\therefore \beta=\frac{C_{0} V}{v}(1-\beta)\left[k_{P}(1-\alpha)+k_{Q}(1-\beta)\right](\mathrm{II})
\end{gathered}
$$

For the single stirred tank, the relative yield of the desired product, $\phi$, is given by the ratio of the rates of reaction; that is,

$$
\phi=\frac{r_{P}}{r_{P}+r_{Q}}=\frac{k_{P} C_{A} C_{B}}{k_{P} C_{A} C_{B}+k_{Q} C_{B}^{2}}=\frac{k_{P} C_{A}}{k_{P} C_{A}+k_{Q} C_{B}}
$$

when, as in the present problem, the reactant proportions are chosen such that $C_{A, 0}$ $=C_{B, 0}=C_{0}$. Accordingly,

$$
\begin{equation*}
\phi=\frac{k_{P} C_{0}(1-\alpha)}{k_{P} C_{0}(1-\alpha)+k_{Q} C_{0}(1-\beta)}=\frac{k_{P}(1-\alpha)}{k_{P}(1-\alpha)+k_{Q}(1-\beta)} \tag{III}
\end{equation*}
$$

For the special case of $k_{P}=k_{Q}=k$, equations (I) and (II) simplify to

$$
\begin{gathered}
\alpha=\frac{k C_{0} V}{v}(1-\alpha)(1-\beta)(\mathrm{IV}) \\
\beta=\frac{k C_{0} V}{v}(1-\beta)(1-\alpha+1-\beta)(\mathrm{V})
\end{gathered}
$$

so that, substituting in (III), we get

$$
\phi=\frac{1-\alpha}{1-\alpha+1-\beta}(\mathrm{VI})
$$

Given the fractional conversion of $\mathrm{B}, \beta=0.95$, we substitute in equations (IV) and (V) to obtain

$$
\begin{gathered}
\alpha=\frac{k C_{0} V}{v}(1-\alpha)(1-0.95) \rightarrow 20 \alpha=\frac{k C_{0} V}{v}(1-\alpha) \text { (VII) } \\
0.95=\frac{k C_{0} V}{v}(1-0.95)(1-\alpha+1-0.95) \rightarrow 19=\frac{k C_{0} V}{v}(1.05-\alpha)(\mathrm{VIII})
\end{gathered}
$$

Dividing equation (VII) by (VIII) gives

$$
\begin{gathered}
\frac{20 \alpha}{19}=\frac{\sum_{v /}^{k C_{0} V /}}{v /} \frac{(1-\alpha)}{(1.05-\alpha)} \rightarrow 1.05 \alpha(1.05-\alpha)=1-\alpha \\
\therefore 1.10 \alpha-1.05 \alpha^{2}=1-\alpha \\
\therefore-1.05 \alpha^{2}+2.10 \alpha-1=0 \\
\therefore \alpha^{2}-2 \alpha+0.952=0
\end{gathered}
$$

Solving the equation above yields $\alpha=0.781$. Inserting this result in equation (VIII) and solving for the reactor volume, we obtain

$$
\begin{gathered}
19=\frac{k C_{0} V}{v}(1.05-\alpha) \rightarrow 19=\frac{k C_{0} V}{v}(1.05-0.781) \\
\therefore 19=\frac{k C_{0} V}{v} \times 0.269 \\
\therefore V=\frac{70.6 v}{k C_{0}}
\end{gathered}
$$

Lastly, the relative yield of P is found by substituting $\alpha$ and $\beta$ into equation (VI),

$$
\phi=\frac{1-0.781}{1-0.781+1-0.95}=0.814
$$

- The correct answer is D.


## P. $8 \rightarrow$ Solution

From the treatment of reactor output given in Volume 3 of Coulson and Richardson's Chemical Engineering, it may be seen that placing the smaller tank first would be an advantage. Bringing the feed into the smaller tank will give a relatively high concentration of reactants in this tank. If the overall order of the reaction is greater than 1 (the overall order being 2 in this example), high concentrations at some stage in the system will lead to higher rates of reaction and larger final fractional conversion compared with any alternative configuration.

The case for preferring the smaller tank first is difficult to sustain however by strictly logical arguments. The most convincing way is to calculate the fractional conversion for both configurations, as the problem suggests.

For a flow of feed of $v \mathrm{~m}^{3} / \mathrm{s}$ with a concentration of either A or B - the concentrations of A and B are equal throughout - of $C_{0} \mathrm{kmol} / \mathrm{m}^{3}$, with the flow passing through tanks of volumes $V_{1}$ and $V_{2}$, then a steady-state mass balance gives, for tank 1,

In - Out - Reaction $=$ Accumulation

$$
\begin{gathered}
\therefore v C_{0}-v\left(C_{0}-a_{1}\right)-V_{1} k\left(C_{0}-a_{1}\right)^{2}=0 \\
\therefore v a_{1}=V_{1} k\left(C_{0}-a_{1}\right)^{2}
\end{gathered}
$$

Here, $a_{1}=X_{1} C_{0}$ is the number of moles of reactant transformed in unit volume of reaction mixture. $X_{1}$ is the fractional conversion. Thus,

$$
\begin{gather*}
v X_{1} C_{0}=V_{1} k C_{0}^{2}\left(1-a_{1}\right)^{2} \\
\therefore X_{1}=\frac{V_{1}}{v} k C_{0}\left(1-X_{1}\right)^{2}(\mathrm{I} \tag{I}
\end{gather*}
$$

Applying a mass balance to tank 2 , in turn, we obtain

$$
\text { In }- \text { Out }- \text { Reaction }=\text { Accumulation }
$$

$$
\begin{gathered}
\therefore v\left(C_{0}-a_{1}\right)-v\left(C_{0}-a_{2}\right)=V_{2} k\left(C_{0}-a_{2}\right)^{2}=0 \\
\therefore v\left(a_{2}-a_{1}\right)=V_{2} k\left(C_{0}-a_{2}\right)^{2} \\
\therefore X_{2}-X_{1}=\frac{V_{2}}{v} k C_{0}\left(1-X_{2}\right)^{2} \quad(\mathrm{II})
\end{gathered}
$$

In both cases, $v=0.3 \times 10^{-3} \mathrm{~m}^{3} / \mathrm{s}, k=1.8 \times 10^{-4} \mathrm{~m}^{3} / \mathrm{kmol} \cdot \mathrm{s}$ and $C_{0}=1.5$
$\mathrm{kmol} / \mathrm{m}^{3}$. In configuration 1, the smaller reactor is placed before the larger one; that is, $V_{1}=30 \mathrm{~m}^{3}$ and $V_{2}=100 \mathrm{~m}^{3}$. Substituting in equation (I), we get

$$
\begin{gathered}
X_{1}=\frac{30}{0.3 \times 10^{-3}} \times\left(1.8 \times 10^{-4}\right) \times 1.5\left(1-X_{1}\right)^{2} \\
\therefore X_{1}=27\left(1-X_{1}\right)^{2} \\
\therefore 27 X_{1}^{2}-55 X_{1}+27=0
\end{gathered}
$$

Solving the equation above, we obtain $X_{1}=0.825$. Applying this result into equation (II) gives

$$
\begin{gathered}
X_{2}-0.825=\frac{100}{0.3 \times 10^{-3}} \times\left(1.8 \times 10^{-4}\right) \times\left(1-X_{2}\right)^{2} \\
\therefore X_{2}-0.825=60\left(1-X_{2}\right)^{2} \\
\therefore 60 X_{2}^{2}-121 X_{2}+60.8=0
\end{gathered}
$$

Solving this equation gives $X_{2}=0.950$. Consider now configuration 2 , in which case the larger reactor comes before the smaller one; that is, $V_{1}=100 \mathrm{~m}^{3}$ and $V_{2}=30 \mathrm{~m}^{3}$. For tank 1, we write

$$
\begin{gathered}
X_{1}=\frac{100}{0.3 \times 10^{-3}} \times\left(1.8 \times 10^{-4}\right) \times 1.5\left(1-X_{1}\right)^{2} \\
\therefore X_{1}=90\left(1-X_{1}\right)^{2} \\
\therefore 90 X_{1}^{2}-181 X_{1}+90=0
\end{gathered}
$$

Solving the equation above, we obtain $X_{1}=0.900$. Substituting in equation (II) yields

$$
\begin{aligned}
X_{2}-0.9 & =\frac{30}{0.3 \times 10^{-3}} \times\left(1.8 \times 10^{-4}\right) \times\left(1-X_{2}\right)^{2} \\
& \therefore 18 X_{2}^{2}-37 X_{2}+18.9=0
\end{aligned}
$$

Solving this equation, $X_{2}=0.948$ is obtained. The results obtained with the two configurations are summarized below.

|  | $\mathrm{X}_{1}$ | $\mathrm{X}_{2}$ |
| :---: | :---: | :---: |
| Configuration 1 <br> (small reactor <br> before large reactor) | 0.825 | 0.95 |
| Configuration 2 <br> (large reactor <br> before small reactor) | 0.9 | 0.948 |

There is seemingly very little difference between the final conversions calculated for the two cases and it may be concluded that, although the final conversion will depend on the total volume of the tanks, it is not very sensitive to how that volume is distributed. In operating a reactor, however, often it is the fraction which is unreacted that is important for downstream separation. In the case at hand, the values are $0.039 \mathrm{kmol} / \mathrm{m}^{3}$ for configuration 1 and $0.045 \mathrm{kmol} / \mathrm{m}^{3}$ for configuration 2.

## P. $9 \rightarrow$ Solution

For the degree of conversion specified, the effluent concentration of benzoquinone must be equal to ( $1-0.9$ ) $\times 0.075=0.0075 \mathrm{kmol} / \mathrm{m}^{3}$. For operation of a single CSTR, the space time is straightforwardly obtained as

$$
\tau=\frac{C_{A, 0}-C_{A, 1}}{k C_{A, 1}^{2}}=\frac{0.075-0.0075}{10.4 \times 0.0075^{2}}=115 \mathrm{ks}
$$

From the definition of space time, the reactor is sized as

$$
\begin{gathered}
\tau=\frac{V}{v_{0}} \rightarrow V=\tau v_{0} \\
\therefore V=115 \times 0.28=32.2 \mathrm{~m}^{3}
\end{gathered}
$$

Suppose now that two identical CSTRs are connected in series. In this case it will be necessary to determine the concentration in the effluent from the first reactor in order to determine the required reactor size. One way of proceeding is to write the design equation for each CSTR. The equations in question are

$$
\frac{V_{R, 1}}{v_{0}}=\frac{C_{B, 0}\left(X_{B, 1}-0\right)}{k C_{B}^{2}\left(1-X_{B, 1}\right)^{2}}
$$

and

$$
\frac{V_{R, 2}}{v_{0}}=\frac{C_{B, 0}\left(X_{B, 2}-X_{B, 1}\right)}{k C_{B, 0}^{2}\left(1-X_{B, 2}\right)^{2}}
$$

Equating the two expressions, we get

$$
\frac{\text { B, }\left(X_{B, 1}-0\right)}{\text { kC }_{B, 0}^{2}\left(1-X_{B, 1}\right)^{2}}=\frac{X_{B, 1}\left(X_{B, 2}-X_{B, 1}\right)}{k C_{B, 2}^{2}\left(1-X_{B, 2}\right)^{2}} \rightarrow \frac{X_{B, 2}-X_{B, 1}}{\left(1-X_{B, 1}\right)^{2}}=\frac{\left.X_{B, 2}\right)^{2}}{\left(1-X_{2}\right.}
$$

Substituting $X_{B, 2}=0.9$ gives

$$
\frac{X_{B, 1}}{\left(1-X_{B, 1}\right)^{2}}=\frac{0.9-X_{B, 1}}{(1-0.9)^{2}}
$$

The result is a third-degree equation in $X_{B, 1}$. Solving it, we obtain $X_{B, 1}=$ 0.763. It follows that $C_{B, 1}=0.075 \times(1-0.763)=0.0178 \mathrm{kmol} / \mathrm{m}^{3}$. We can now return to either of the design equations and establish the size of the reactor,

$$
V_{R, 1}=\frac{v_{0} C_{B, 0} X_{B, 1}}{k C_{B, 0}^{2}\left(1-X_{B, 1}\right)^{2}}=\frac{0.28 \times 0.075 \times 0.763}{10.4 \times 0.075^{2} \times(1-0.763)^{2}}=4.88 \mathrm{~m}^{3}
$$

The total volume of the two reactors is $2 \times 4.88=9.76 \mathrm{~m}^{3}$, which is considerably less than the volume required if a single CSTR were used.

Consider now a cascade of three CSTRs. In this case there are two intermediate unspecified reactant concentrations instead of just the single intermediate concentration encountered in the previous section. At least one of these concentrations must be determined if one is able to size the reactors appropriately. In principle, one may follow the procedure used in the previous part whereby one writes the design equations for each CSTR and then equates the reactor space times. This procedure gives three equations and three unknowns namely, reactor size $V_{R, 1}$ and conversions $X_{B, 1}$ and $X_{B, 2}$. Thus, for the first reactor,

$$
\frac{V_{R, 1}}{v_{0}}=\frac{C_{B, 0}\left(X_{B, 1}-0\right)}{k C_{B, 0}^{2}\left(1-X_{B, 1}\right)^{2}}
$$

For the second reactor,

$$
\frac{V_{R, 2}}{v_{0}}=\frac{C_{B, 0}\left(X_{B, 2}-X_{B, 1}\right)}{k C_{B, 0}^{2}\left(1-X_{B, 2}\right)^{2}}
$$

and for the third,

$$
\frac{V_{R, 3}}{v_{0}}=\frac{C_{B, 0}\left(0.9-X_{B, 2}\right)}{k C_{B, 0}^{2}(1-0.9)^{2}}
$$

Combining the first and third equations gives

$$
\begin{gathered}
\frac{\text { C, } X_{B, 1}}{\left.2, X_{B, 1}\right)^{2}}=\frac{\left(1-X_{B, 2}\right)}{k, C_{B, 0}^{2}(1-0.9)^{2}} \\
\therefore \frac{X_{B, 1}}{\left(1-X_{B, 1}\right)^{2}}=\frac{\left(0.90-X_{B, 2}\right)}{0.01} \\
\therefore X_{B, 2}=0.9-\frac{0.01 X_{B, 1}}{\left(1-X_{B, 1}\right)^{2}}(\mathrm{I})
\end{gathered}
$$

Combining the first and second equation, in turn, gives

$$
\begin{gathered}
\frac{\text { B, }\left(X_{B, 1}-0\right)}{\text { k, }\left(1-X_{B, 1}\right)^{2}}=\frac{\left.X_{B, 2}^{2}-X_{B, 1}\right)}{2\left(1-X_{B, 2}\right)^{2}} \\
\therefore \frac{X_{B, 1}}{\left(1-X_{B, 1}\right)^{2}}=\frac{X_{B, 2}-X_{B, 1}}{\left(1-X_{B, 2}\right)^{2}}
\end{gathered}
$$

Replacing $X_{B, 2}$ with the result from equation (I) yields

$$
\begin{gathered}
\frac{X_{B, 1}}{\left(1-X_{B, 1}\right)^{2}}=\frac{X_{B, 2}-X_{B, 1}}{\left(1-X_{B, 2}\right)^{2}} \\
\therefore \frac{X_{B, 1}}{\left(1-X_{B, 1}\right)^{2}}=\frac{0.9-0.01 X_{B, 1} /\left(1-X_{B, 1}\right)^{2}-X_{B, 1}}{\left[1-0.9+0.01 X_{B, 1} /\left(1-X_{B, 1}\right)^{2}\right]^{2}}
\end{gathered}
$$

Solving the equation above yields $X_{B, 1}=0.672$. Substituting this result into (I) gives the other conversion we are looking for

$$
X_{B, 2}=0.9-\frac{0.01 \times 0.672}{(1-0.672)^{2}}=0.838
$$

Having obtained the conversions, we can establish the volume of the reactor with any of the design equations,

$$
V_{R, 1}=\frac{v_{0} C_{B, 0} X_{B, 1}}{k C_{B, 0}^{2}\left(1-X_{B, 1}\right)^{2}}=\frac{0.28 \times 0.075 \times 0.672}{10.4 \times 0.075^{2} \times(1-0.672)^{2}}=2.24 \mathrm{~m}^{3}
$$

The total volume of the cascade is then $3 \times 2.24=6.72 \mathrm{~m}^{3}$, which is again a significant reduction in the volume requirement, but not nearly as great as that brought about in going from one to two CSTRs in series.

- The correct answers are 1-C, 2-D and 3-B.


## P. $10 \rightarrow$ Solution

1. True. The PFR volume is given by the area below the Levenspiel plot from $X=0$ to $X=0.5$, as shown.

$$
\frac{\mathrm{F}_{\mathrm{A} 0}}{-\mathrm{r}_{\mathrm{A}}}\left(\mathrm{~m}^{3}\right)_{200,000}^{500,000}
$$

Accordingly,

$$
\begin{gathered}
V_{P F R}=\text { Area }_{\text {Rectangle A }}+\text { Area }_{\text {Triangle } \mathrm{B}} \\
\therefore V_{P F R}=0.5 \times 100,000+\frac{1}{2} \times 0.5 \times(500,000-100,000)=150,000 \mathrm{~m}^{3}
\end{gathered}
$$

2. False. The CSTR volume is given by the rectangle shown below.


In mathematical terms,

$$
V_{C S T R}=\mathrm{Area}_{\text {Rectangle A }}=0.5 \times 100,000=50,000 \mathrm{~m}^{3}
$$

3. True. We first draw two vertical lines, one beginning at a conversion $X=$ 0.5 and another at $X=0.8$, which is the conversion we aim for. The volume of the additional CSTR is given by the rectangle encompassed by the two lines, as shown.


Mathematically,

$$
V_{C S T R}=\text { Area }_{\text {Rectangle } \mathrm{A}}=(0.8-0.5) \times 500,000=150,000 \mathrm{~m}^{3}
$$

4. False. As we did in the previous part, a vertical line is drawn at conversion values $X=0.5$ and $X=0.8$. Since we are dealing with a PFR, the volume is given by the shaded area below the Legenspiel plot, as shown.


$$
\begin{gathered}
V_{P F R}=\mathrm{Area}_{\text {Rectangle } \mathrm{A}}+\text { Area }_{\text {Triangle } \mathrm{B}} \\
\therefore V_{P F R}=(0.8-0.5) \times 100,000+\frac{1}{2} \times(0.8-0.5) \times(500,000-100,000)=90,000 \mathrm{~m}^{3}
\end{gathered}
$$

## P. $11 \rightarrow$ Solution

1.True. To begin, we prepare a table with the values of $1 /\left(-r_{A}\right)$.

| $X$ | 0 | 0.2 | 0.4 | 0.45 | 0.5 | 0.6 | 0.8 | 0.9 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $-r_{A}\left(\mathrm{~mol} / \mathrm{dm}^{3} \cdot \mathrm{~min}\right)$ | 1.0 | 1.67 | 5.0 | 5.0 | 5.0 | 5.0 | 1.25 | 0.91 |
| $1 /\left(-r_{A}\right)\left(\mathrm{dm}^{3} \cdot \mathrm{~min} / \mathrm{mol}\right)$ | 1.0 | 0.6 | 0.2 | 0.2 | 0.2 | 0.2 | 0.8 | 1.10 |

The Levenspiel plot is outlined below


We are looking for the PFR volume needed to achieve 40\% conversion. This is given by the integral

$$
V_{P F R}=F_{A, 0} \int_{0}^{0.4} \frac{d X}{-r_{A}}
$$

Appealing to Simpson's three-point rule, we have

$$
V_{P F R}=F_{A, 0}\left\{\frac{\Delta X}{3}\left[\left(\frac{1}{-r_{A}}\right)_{X=0}+4\left(\frac{1}{-r_{A}}\right)_{X=0.2}+\left(\frac{1}{-r_{A}}\right)_{X=0.4}\right]\right\}
$$

The step length is $\Delta X=(0.4-0) / 2=0.2$. Substituting in the equation above brings to

$$
V_{P F R}=300 \times\left[\frac{0.2}{3} \times(1.0+4 \times 0.599+0.2)\right]=71.9 \mathrm{dm}^{3}
$$

2.False. The volume of CSTR required for the same conversion is straightforwardly obtained as

$$
V_{C S T R}=\frac{F_{A, 0} X}{-r_{A}}=300 \times 0.4 \times 0.2=24 \mathrm{dm}^{3}
$$

3.False. The conversion achieved by a $72-\mathrm{dm}^{3}$ PFR, as established in the analysis of Statement 1 , is about $X_{1} \approx 0.4$. It remains to compute the conversion $X_{2}$ obtained by the CSTR, which is given by

$$
\begin{gathered}
V=\left(\frac{F_{A, 0}}{-r_{A}}\right)_{X_{2}}\left(X_{2}-X_{1}\right) \rightarrow \frac{\left(X_{2}-X_{1}\right)}{-r_{A}}=\frac{V}{F_{A, 0}} \\
\therefore \frac{\left(X_{2}-X_{1}\right)}{-r_{A}}=\frac{24}{300}=0.08
\end{gathered}
$$

We proceed by trial-and-error. At $X_{2}=0.4$, with reference to the Legenspiel plot, the value of $-r_{A}=1 / 0.2=5$. Thus,

$$
\frac{\left(X_{2}-X_{1}\right)}{-r_{A}}=\frac{(0.6-0.4)}{5}=0.04 \neq 0.08
$$

The values do not match. Suppose instead that $X_{2}=0.65$. Referring to the chart, we read $-r_{A}=1 / 0.35=2.86$. It follows that

$$
\frac{\left(X_{2}-X_{1}\right)}{-r_{A}}=\frac{(0.65-0.4)}{2.86}=0.0874 \approx 0.08
$$

The values are close enough, and we conclude that the conversion achieved by a $72-\mathrm{dm}^{3}$ PFR followed by a $24-\mathrm{dm}^{3}$ CSTR is 0.65 .
4.True. The analysis of Statement 2 shows that the conversion achieved by a $24-\mathrm{dm}^{3}$ CSTR is about 0.4. The next step is to determine the conversion associated with the PFR. Let the outlet conversion of the PFR be 0.8. From Simpson's three-point rule, we write

$$
V=F_{A, 0}\left\{\frac{\Delta X}{3}\left[\left(\frac{1}{-r_{A}}\right)_{X=0.4}+4\left(\frac{1}{-r_{A}}\right)_{X=0.6}+\left(\frac{1}{-r_{A}}\right)_{X=0.8}\right]\right\}
$$

The step length is $\Delta X=(0.8-0.4) / 2=0.2$. Substituting, we get

$$
V=300 \times\left[\frac{0.2}{3} \times(0.2+4 \times 0.2+0.8)\right]=36 \mathrm{dm}^{3}
$$

This value of $V$ does not match the volume of the PFR, and another trial is in order. In a second iteration, let $X_{2}=0.9$. Applying Simpson's three-point rule again, we write

$$
V=F_{A, 0}\left\{\frac{\Delta X}{3}\left[\left(\frac{1}{-r_{A}}\right)_{X=0.4}+4\left(\frac{1}{-r_{A}}\right)_{X=0.65}+\left(\frac{1}{-r_{A}}\right)_{X=0.9}\right]\right\}
$$

The step length is now $\Delta X=(0.9-0.4) / 2=0.25$. Thus,

$$
V=300 \times\left[\frac{0.25}{3} \times(0.2+4 \times 0.35+1.1)\right]=67.5 \mathrm{dm}^{3}
$$

The result is closer to $72 \mathrm{dm}^{3}$ but not quite there yet. In a third iteration, let $X_{2}=0.91$. In this case,

$$
V=F_{A, 0}\left\{\frac{\Delta X}{3}\left[\left(\frac{1}{-r_{A}}\right)_{X=0.4}+4\left(\frac{1}{-r_{A}}\right)_{X=0.655}+\left(\frac{1}{-r_{A}}\right)_{X=0.91}\right]\right\}
$$

The step length is now $\Delta X=(0.91-0.4) / 2=0.255$. Interpolating between points $\{0.6,0.2\}$ and $\{0.8,0.8\}$, we get $1 /\left(-r_{A}\right)=0.365$ at $X=0.655$. Extrapolating between the same points, we obtain $1 /\left(-r_{A}\right)=1.13$ at $X=0.91$. Thus,

$$
V=300 \times\left[\frac{0.255}{3} \times(0.2+4 \times 0.365+1.13)\right]=71.1 \mathrm{dm}^{3}
$$

This value is quite close to the actual volume of the PFR. We conclude that the conversion achieved by a $72-\mathrm{dm}^{3}$ PFR followed by a $24-\mathrm{dm}^{3}$ CSTR is 0.91 .

ANSWER SUMMARY

| Problem 1 | D |
| :---: | :---: |
| Problem 2 | C |
| Problem 3 | B |
| Problem 4 | A |
| Problem 5 |  |
| Problem 6 |  |
| Problem 7 |  |
| Problem 8 |  |
| Problem 9 | B |
|  | 9.1 |
|  | Problem 10 |  |
| Problem 11 |  |
|  |  |

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