Conversion in Non-Ideal Flow Reactors

$$\begin{pmatrix}\text{mean concentration}\\ \text{of reactant}\\ \text{in exit stream}\end{pmatrix} = \sum_{\substack{\text{all elements}\\ \text{of exit stream}}} \begin{pmatrix}\text{concentration of}\\ \text{reactant remaining}\\ \text{in an element of}\\ \text{age between } t\\ \text{and } t+dt\end{pmatrix}\begin{pmatrix}\text{fraction of exit}\\ \text{stream which is}\\ \text{of age between } t\\ \text{and } t+dt\end{pmatrix}$$

$$\left(\frac{\overline{C}_A}{C_{A0}}\right)_{\text{at exit}} = \int_0^\infty \left(\frac{C_A}{C_{A0}}\right)_{\substack{\text{for an element or little}\\ \text{batch of fluid of age } t}} \cdot \mathbf{E}\, dt$$

Conversion in Non-Ideal Flow Reactors

- Conversion at the reactor exit is the sum of the concentration of reactant remaining in an element multiplied by the fraction of exit between t and t+dt.
- This is represented mathematically by:

$$\left(\frac{\overline{C}_A}{C_{A0}}\right)_{\text{at exit}} = \int_0^\infty \left(\frac{C_A}{C_{A0}}\right)_{\substack{\text{for an element or little}\\ \text{batch of fluid of age } t}} \cdot \mathbf{E}\, dt \qquad \textbf{(1)}$$

$$\overline{X}_A = \int_0^\infty (X_A)_{\text{element}} \cdot \mathbf{E}\, dt \qquad \textbf{(2)}$$

or in a form suitable for numerical integration

$$\frac{\overline{C}_A}{C_{A0}} = \sum_{\substack{\text{all age}\\ \text{intervals}}} \left(\frac{C_A}{C_{A0}}\right)_{\text{element}} \cdot \mathbf{E}\, \Delta t \qquad \textbf{(3)}$$

Conversion in Non-Ideal Flow Reactors (cont.)

- In equation one, the concentration element term is dependent on the order of the reaction.

1st-Order Reactions:

$$\left(\frac{C_A}{C_{AO}}\right)_{element} = e^{-kt}$$

2nd-Order Reactions:

$$\left(\frac{C_A}{C_{AO}}\right)_{element} = \frac{1}{1 + kC_{AO}t}$$

Conversion in Non-Ideal Flow Reactors (cont.)

- Finally, the following termed can be applied to equation 1 for any order reaction.

nth-Order Reactions:

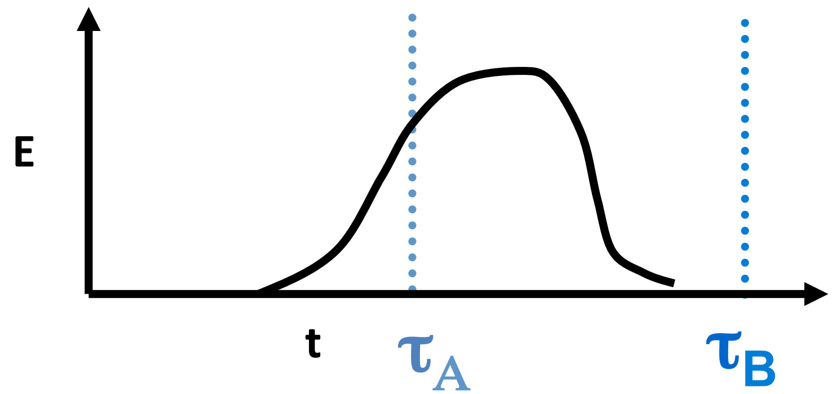
$$\left(\frac{C_A}{C_{AO}}\right)_{element} = [1+(n-1)C_{AO}^{n-1}kt]^{\frac{1}{1-n}}$$

Conversion in Non-Ideal Flow vs. Ideal Flow Reactors

- The space time parameter, τ, is equal to the reactor volume divided by the volumetric feed rate. τ is an important parameter in calculating conversion in ideal flow reactors.

- Where τ falls on the x-axis of an E(t) curve indicates how much more or less conversion is occurring in a non-ideal reactor as compared to an ideal reactor.

Conversion in Non-Ideal Flow vs. Ideal Flow Reactors (cont.)



- Case A: Particles are spending more time than expected in the reactor. Therefore, a higher conversion is being achieved in a non-ideal situation than would be in an ideal situation.

- Case B: Particles are spending less time than expected in the reactor. Therefore, a lower conversion is being achieved in a non-ideal situation than would be in an ideal situation.

Example 11.4: Determining Conversion in Non-Ideal Reactors

- Problem Statement: A liquid is decomposing in a non-ideal reactor in Example 11.1 at a rate which can be expressed by $-r_A = kC_A$ where $k = 0.307\ \text{min}^{-1}$.

- Determine: Fraction of reactant unconverted in the real reactor and compare this with the fraction unconverted in a plug flow reactor of the same size.

For the *plug flow reactor* with negligible density change we have

$$\tau = C_{A0} \int_0^{X_A} \frac{dX_A}{-r_A} = -\frac{1}{k} \int_{C_{A0}}^{C_A} \frac{dC_A}{C_A} = \frac{1}{k} \ln \frac{C_{A0}}{C_A}$$

and with τ from Example 11.1

$$\frac{C_A}{C_{A0}} = e^{-k\tau} = e^{-(0.307)(15)} = e^{-4.6} = \underline{\underline{0.01}}$$

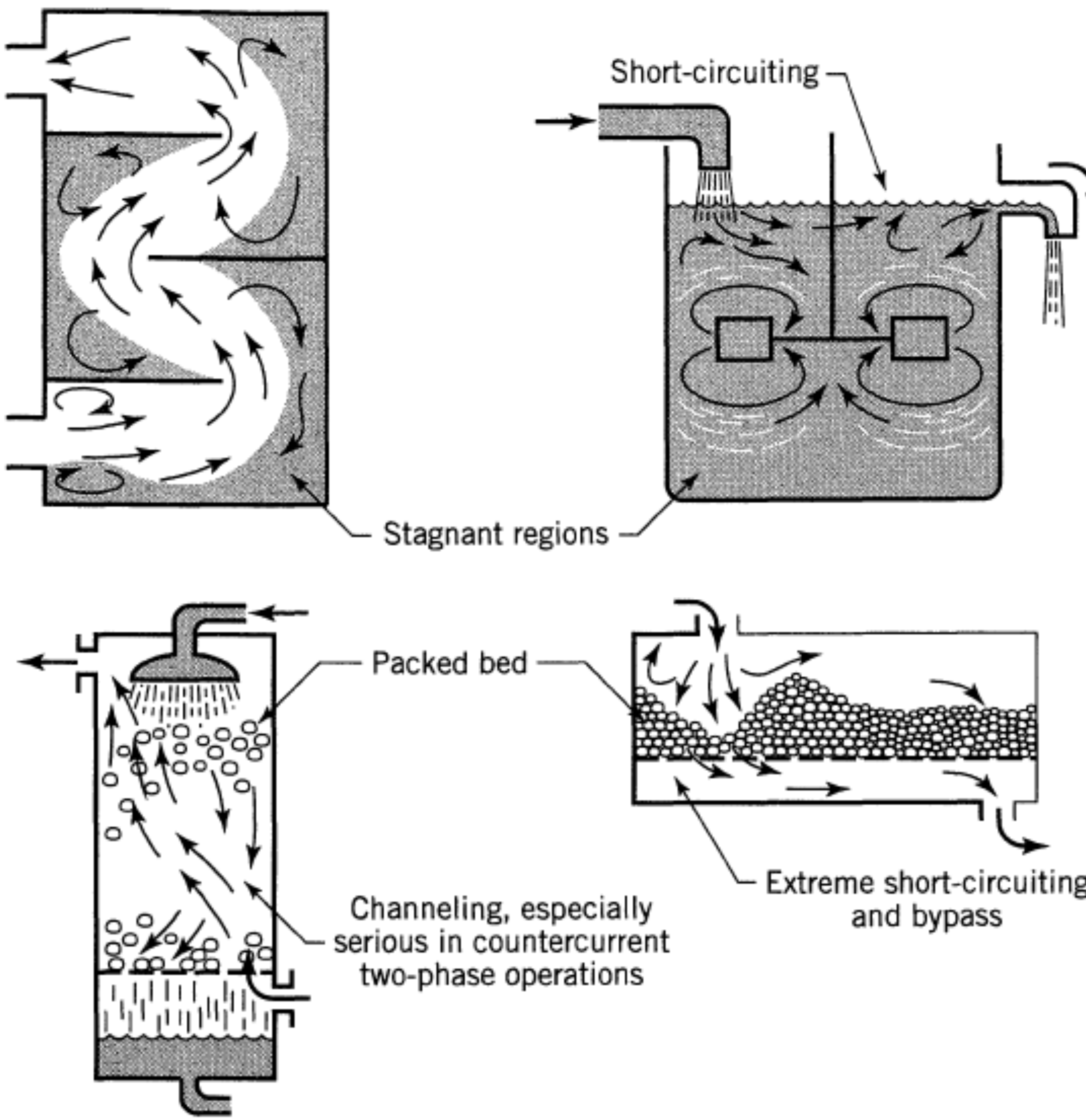
Thus the fraction of reactant unconverted in a plug flow reactor equals 1.0%.

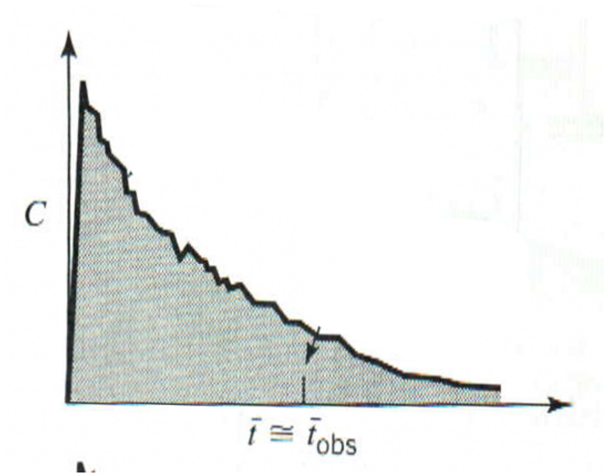
Table E11.4

t	$\mathbf{E}$	kt	e^{-kt}	$e^{-kt}\mathbf{E}\,\Delta t$
5	0.03	1.53	0.2154	$(0.2154)(0.03)(5) = 0.0323$
10	0.05	3.07	0.0464	0.0116
15	0.05	4.60	0.0100	0.0025
20	0.04	6.14	0.0021	0.0004
25	0.02	7.68	0.005	0.0001
30	0.01	9.21	0.0001	0
given				$\dfrac{C_A}{C_{A0}} = \sum e^{-kt}\mathbf{E}\,\Delta t = \underline{\underline{0.0469}}$

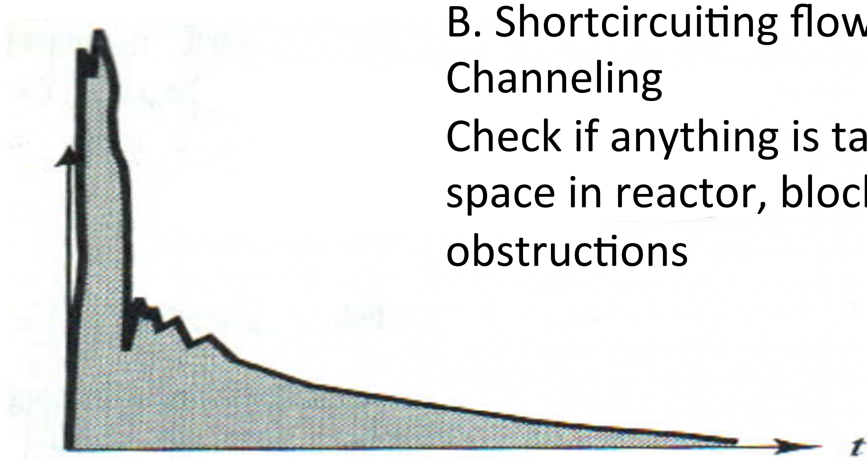
$$\frac{C_A}{C_{A0}} = \underline{\underline{0.047}}$$

From the table we see that the unconverted material comes mostly from the early portion of the E curve.


Short-circuiting
Stagnant regions
Packed bed
Channeling, especially serious in countercurrent two-phase operations
Extreme short-circuiting and bypass



A. Normal MFR



B. Shortcircuiting flow/
Channeling
Check if anything is taking up space in reactor, blockages/ obstructions