

Kostuv Ray Qs

1. Residence Time, Space Velocity, Space Time

Residence Time(Space Time): The total time a particle spends inside a control volume. (chemical reactor in this case)

Space Time: Time necessary to process one reactor volume feed at the entrance conditions.

$$\tau = \frac{V}{V_0} = \frac{VC_{A0}}{F_{A0}}$$

Space Velocity (Space Time Inverse): How many reactor volumes of feed can be fed in unit time?

$$S_v = \frac{1}{\tau} = \frac{\text{Volumetric Flow Rate}}{\text{Volume}}$$

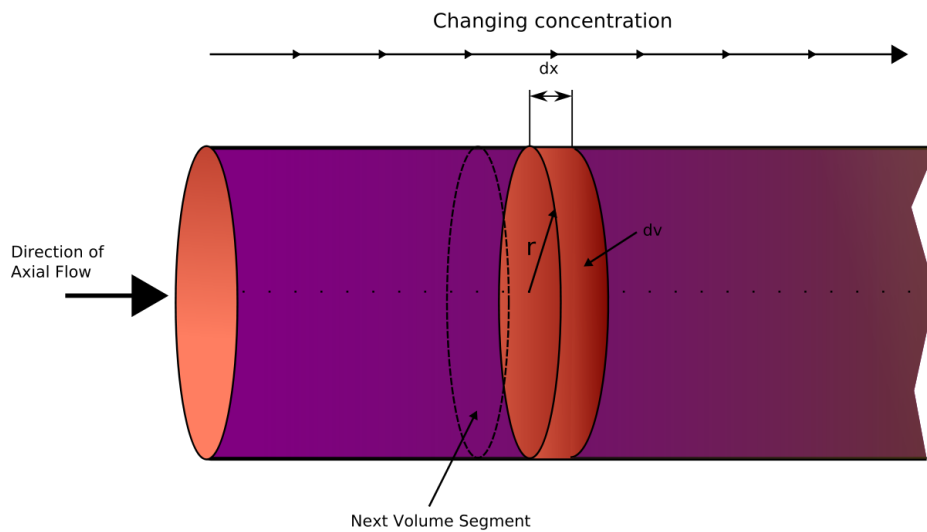
2. Types of Reactors

- **Batch:**
- **Plug Flow Reactors:**

○ Material Balance: $V = \int_0^{X_A} \frac{F_{A0}}{-r_A} dX_A$ **OR**

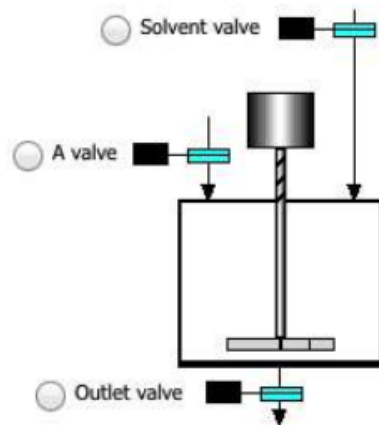
$$V \frac{dC_A}{dV} = -kC_A$$

○ $\tau = C_{A0} \int_0^X \frac{DX}{-r_A}$



- **Continuous Stirred Tank Reactors:**

- Material Balance: $V = \frac{F_{A0}}{-r_A} X_A$
- Conversion Equation: $X = 1 - \frac{1}{(1+\tau k)^n}$



3. CSTR Vs. PFR

CSTR maintains the same concentration at any point in the reactor while PFR has only radial mixing. CSTR reduces the concentration of reactant to a minimum of less than what PFR does.

4. What is reactor design?

Reactor design is necessary to minimize waste, energy consumption, catalyst depletion, and other raw materials usage.

5. Why multiple reactors in series are preferred over a single reactor in certain situations?

CSTRs in series are used fairly commonly to reduce the total reactor volume required while retaining the advantages of CSTR.

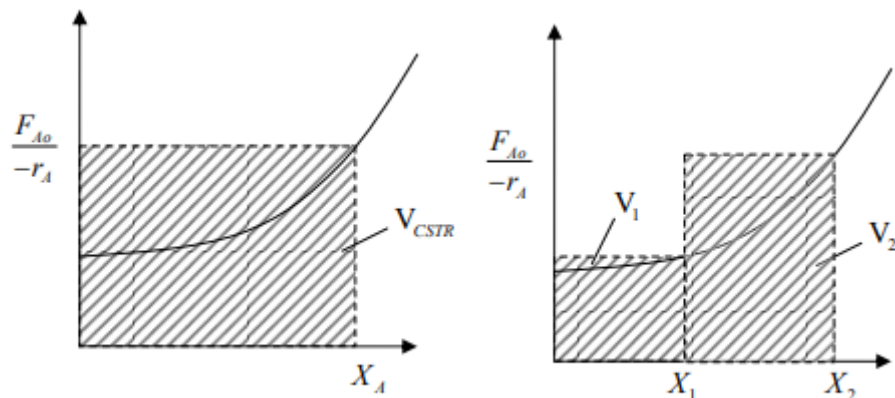
Derivation:

$$V_1 = \frac{F_{A0}}{-r_{A_1}} X_1$$

Material Balance (In + Out + Prod = Acc = 0)

$$F_{A_1} - F_{A_2} + r_{A_2} V_2 = \text{Steady State}$$

$$F_{A_2} = F_{A_0} - X_2 F_{A_0} \Rightarrow V_2 = \frac{F_{A_0}}{-r_{A_2}} (X_2 - X_1)$$



Levenspiel Plots

PFR in series has no change in conditions between reactors, the total PFR volume will be the same as the volume of one PFR operating at the same conversion.

6. When would we prefer to use CSTRs in parallel?

When there is a large pressure drop in the reactor, using CSTRs in parallel is more economical than setting up a very long CSTR.

7. Assumptions are considered in the analysis of ideal CSTR and PFR.

- CSTR:
 - Perfect Mixing
 - Steady State
 - Constant Temperature
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 - Closed boundaries
 - Constant Fluid Density
 - Alright for liquids
 - Doesn't work for most polymerization reactions

- Gases: As long as there is no net change in no. of moles ($dN_A = 0$) & ($dT = 0$)

- **PFR**

- Plug Flow: Constant velocity across a cross-section.
- Fluid is perfectly mixed in the radial direction.
- Steady State
- Constant Density

8. Velocity profile along the axial length in PFR

9. What is the effectiveness factor?

The ratio of the real reaction rate of the catalyst particle to the imaginary reaction rate when the whole particle is assumed to bathe in the surface reactant concentration (ideal scenario).

10. Range of effectiveness in heterogeneous catalytic reactions?

11. Can the effectiveness factor be greater than 1 in the case of exothermic and endothermic reactions?

12. What is fugacity? Is fugacity a physical property?

It is the effective partial pressure that replaces the mechanical partial pressure of its ideal counterpart in an accurate computation of the chemical equilibrium constant.

It is equal to the pressure of an **ideal gas** which has the same temperature and molar **Gibbs free energy** as the real gas.

NO, fugacity is a calculated property.

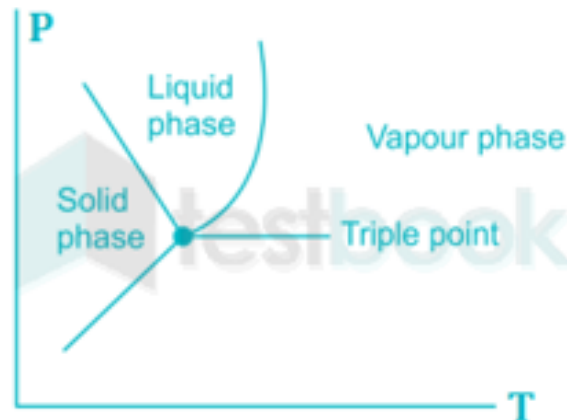
13. Relationship of fugacity and chemical potentials, and why fugacity is used?

The fugacity of gas in any system is a measure of the difference between its chemical potential in that system and its chemical potential in its hypothetical ideal-gas standard state at the same time.

14. Calculate epsilon for a given reaction $2A \rightarrow B$, where 50% A and 50% Inert was present initially

15. Degree of freedom of Triple point (Ans 0)

Degrees of Freedom: No. of variables that can be changed without changing the identity of the phases in equilibrium.



Gibbs Phase Rule:

$$P + F = C + 2$$

P= No. of phases, F= Degree of Freedom, C= No. of components
For pure substances, C=1 & P=3 at the triple point.

16. Calculate epsilon (Expansion Factor) for a given reaction $2A \rightarrow B$, where 50% A and 50% Inert was present initially

Let Initial no. of Moles = 100

Initial no. of moles: A=50, I=50, B=0.
Total Initial no. of moles=100

Final Composition: A=0, I=50, B=25 = 75 mol total

Expansion Factor = $(75-100)/100$

17. Relation between conversation rate if we keep cstr then pfr and if pfr then cstr for 0/1st/2nd order

0 & 1st Order: The order doesn't matter

Proof (1st order)

First, let's take CSTR followed by PFR.

$$0 = VC_{A_0} - VC_{A_1} - kC_{A_1}V_C$$

$$C_{A_1} = \frac{VC_{A_0}}{V + kV_C} \text{ Next, we have } V \frac{dC_A}{dV} = -kC_A$$

$$\int_{C_{A_1}}^{C_{A_2}} \frac{dC_A}{C_A} = - \int_0^{V_P} k \frac{dV}{V} \Rightarrow \ln\left(\frac{C_{A_2}}{C_{A_1}}\right) = - \frac{kV_P}{V}$$

$$C_{A_2} = C_{A_1} e^{-\frac{kV_P}{V}} = \frac{VC_{A_0}}{V+kV_C} e^{-\frac{kV_P}{V}}$$

Next, we have PFR followed by CSTR

$$V \frac{dC_A}{dV} = -kC_A \Rightarrow \ln\left(\frac{C_{A_1}}{C_{A_0}}\right) = -\frac{kV_P}{V} \Rightarrow C_{A_1} = C_{A_0} e^{-\frac{kV_P}{V}}$$

Now, we have CSTR $C_{A_2} = \frac{VC_{A_1}}{V+kV_C} = \frac{VC_{A_0}}{V+kV_C} e^{-\frac{kV_P}{V}}$

18. Types of diffusion

- Molecular Diffusion:

$$\circ J_A = -D_{AB} \frac{dC_A}{dx} = -\frac{D_{AB} C_A}{RT} \frac{du_A}{dx}$$

- Surface Diffusion: Movement along surface

$$\circ J_A = -D_S \frac{dC_A}{dx} \text{ where } D_S \text{ is surface diffusivity}$$

- Knudsen Diffusion: (Catalyst)

$$\circ \text{Occurs when } d_{pore} < \lambda (\text{mean free path})$$

$$\circ k_n = \frac{\lambda}{d_{pore}} (\text{Knudsen Number})$$

$$\blacksquare k_n > 1 \text{ Knudsen Diffusion Occurs}$$

$$\circ J_A = -\frac{D_{kA}}{\tau} \epsilon \frac{dC_A}{dx}$$

$$\blacksquare \epsilon: \text{Porosity Correction Factor} = \frac{V_{eff}}{V_{Total}}$$

$$\blacksquare \tau: \text{Tortuosity} = \frac{\text{Torturous Length}}{\text{Actual Length}}$$

- When both molecular & knudsen diffusion occurring

$$\circ \frac{1}{D} = \frac{1}{D_{KA}} + \frac{1}{D_{AB}} \text{ where } D \text{ is the effective diffusivity}$$

- Eddy Diffusion: (Convective Mass Transfer)

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