Solution to Workshop 01 - Mole balances

Lecture notes for chemical reaction engineering

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> **Note**
>
> Handwritten solutions to these problems are uploaded at Workshop 1 solutions

Q 1-5

What assumptions were made in the derivation of the design equation for:

(a) The batch reactor (BR)?
(b) The CSTR?
(c) The plug-flow reactor (PFR)?
(d) The packed-bed reactor (PBR)?
(e) State in words the meanings of $-r_A$ and $-r'_A$.

Solution

Batch reactor

1. **Perfect mixing:** The reactor contents are perfectly mixed (Ideal reactor).
2. **Constant Volume**: The reactor volume is constant.
3. **Constant Physical Properties**: The physical properties (density, viscosity, etc.) of the reaction mixture are constant.
4. **Single Reaction Phase**: The reaction is assumed to occur in a single phase (either all gas, all liquid, or all solid).
5. **Closed system**: No material is lost to the surroundings.

Continuously Stirred Tank Reactor (CSTR)

1. **Steady-State Operation**: No accumulation of reactants or products over time.
2. **Continuous Flow:** Material continuously flows into and out of the reactor.
3. **Perfect mixing**: The composition is uniform throughout the reactor.

4. **Constant Volume**: The volume of fluid within reactor remains constant.
5. **Constant Physical Properties**

Plug-flow reactor (PFR)

1. **Steady-State Operation**: no accumulation of materials in any section of the reactor over time.
2. **Plug Flow**: The flow through the reactor is plug flow, meaning all elements of the fluid move with the same velocity and there's no back-mixing.
3. **Constant Cross-Sectional Area**: The cross-sectional area of the PFR is constant along its length.
4. **One-Dimensional Flow**: The flow of reactants and products is considered only in the axial direction, ignoring effects in the radial or circumferential directions. Concentration and temperature changes along the length of the reactor not radially.
5. **No pressure drop**; **Constant Physical Properties**

Packed-bed reactor (PBR)

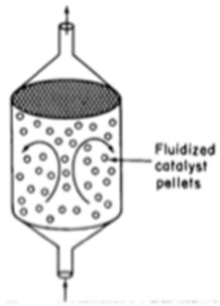
1. **Steady-State Operation**
2. **One-Dimensional Flow**
3. **No pressure drop**; **Constant Physical Properties**
4. **No Back-Mixing**: The reactor operates under plug flow conditions with no back-mixing or axial dispersion of reactants or products.
5. **Constant Cross-Sectional Area**: The cross-sectional area of the PFR is constant along its length.
6. **Uniform Packing**: Constant surface area for reaction per unit reactor volume.

State in words the meanings of $-r_A$ and $-r'_A$.

$-r_A$ is the moles of A reacted per unit volume of reactor per unit time. It is based on the volume of the reactor and has units of $mol/dm^3\ s$. Whereas, $-r'_A$ is the number of moles of A reacted per unit mass of catalyst per unit time. It based on the mass of the catalyst and has units of $mol/kg - cat\ s$. $-r_A$ is used for homogeneous reactions, $-r'_A$ is used for heterogeneous reactions involving solid catalysts.

Q 1-6

Use the mole balance to derive an equation analogous to Equation (1-7) ($V = (F_j0 - F_j)/ - r_j$) for a fluidized CSTR containing catalyst particles (Figure 1) in terms of the catalyst mass, W, and other appropriate terms.



$$W = \frac{F_{A0} - F_A}{-r'_A} \qquad \text{(Q1-6)}$$

Figure Q1-6 Fluidized Bed CSTR.

Figure 1: fig-q1.6

Solution

Assumptions:

1. Steady state
2. Completely mixed: As the catalyst particles rigorously mix within fluidized bed.

Since the reaction occurs on the catalyst, we take mass of catalyst as basis and not the volume of the fluidized bed. Thus for component j the rate is expressed as r'_j with unit $mol/kg - cat\ s$.

General mole balance:

$$F_{j0} - F_j + \int^V \rho_b r'_j dV = \frac{dN_j}{dt} \tag{1}$$

Since the reactor is at steady state

$$\frac{dN_j}{dt} = 0 \tag{2}$$

completely mixed assumption means

$$\int^V \rho_b r'_j dV = \rho_b V r'_j \tag{3}$$

The weight of catalyst W can be written as

$$W = \rho_b V \tag{4}$$

where, ρ_b is the bulk density.

The mole balance equation thus becomes

$$F_{j0} - F_j + W r'_j = 0 \tag{5}$$

Rearranging

$$W = \frac{F_j - F_{j0}}{r'_j} \tag{6}$$

P 1.4 LA Basin

Solution to the LA Basin problem

P 1-5

The reaction A $\longrightarrow$ B is to be carried out isothermally in a continuous-flow reactor. The entering volumetric flow rate v_0 is $10dm^3/h$. (Note: $F_A = C_A v$. For a constant volumetric flow rate $v = v_0$, then $F_A = C_A v_0$. Also, $C_{A0} = F_{A0}$ / v_0 = ([$5mol/h$] / [$10dm^3/h$]) $= 0.5mol/dm^3$.)

Calculate both the CSTR and PFR reactor volumes necessary to consume 99% of A (i.e., $C_A = 0.01C_{A0}$) when the entering molar flow rate is $5mol/h$, assuming the reaction rate $-r_A$ is

a). $-r_A = k$ with $k = 0.05mol/h \cdot dm^3$ b). $-r_A = kC_A$ with $k = 0.0001s^{-1}$ c). $-r_A = kC_A^2$ with $k = 300dm^3/mol \cdot h$ d). Repeat (a), (b), and/or (c) to calculate the time necessary to consume 99.9% of species A in a $1000dm^3$ constant-volume batch reactor with $C_{A0} = 0.5mol/dm^3$.

Solution

Reaction:

A $\longrightarrow$ B

Assumptions:

- Isothermal
- Continuous flow reactor

Data:

υ_0 (dm^3/h) = 10

C_{A0} (mol/dm^3) = 0.5

X = 0.99

Question a

$-r_A = k$

k = 0.05 mol/h dm^3

For CSTR,

$$V = \frac{F_{A0} - F_A}{-r_A} \tag{7}$$

Where, $F_{A0} = C_{A0}\upsilon$

$$F_A = C_A\upsilon$$

F_A = 0.01 $C_{A0}\upsilon$

From Data

F_{A0} = 5.00 mol/h; F_A = 0.05 mol/h

$\therefore V_{CSTR}$ = 99.00 dm^3.

For PFR,

$$\frac{dF_A}{dV} = r_A$$

$$F_A = C_A\upsilon_0; F_{A0} = C_{A0}\upsilon_0$$

$$-r_A = k$$

$$\frac{dC_A\upsilon_0}{dV} = -k$$

$$\frac{\upsilon_0}{-k}\int_{C_{A0}}^{C_A} dC_A = \int_0^V dV$$

$$V = \frac{\upsilon_0}{k}\left(C_{A0} - C_A\right)$$

$\therefore V_{PFR}$ = 99.00 dm^3.

Other question can be solved on the same lines.

Final answers:

b. $V_{CSTR} = 2750\, dm^3; V_{PFR} = 127.9\, dm^3$
c. $V_{CSTR} = 660\, dm^3; V_{PFR} = 6.6\, dm^3$
d. Batch reactor: 66600 h