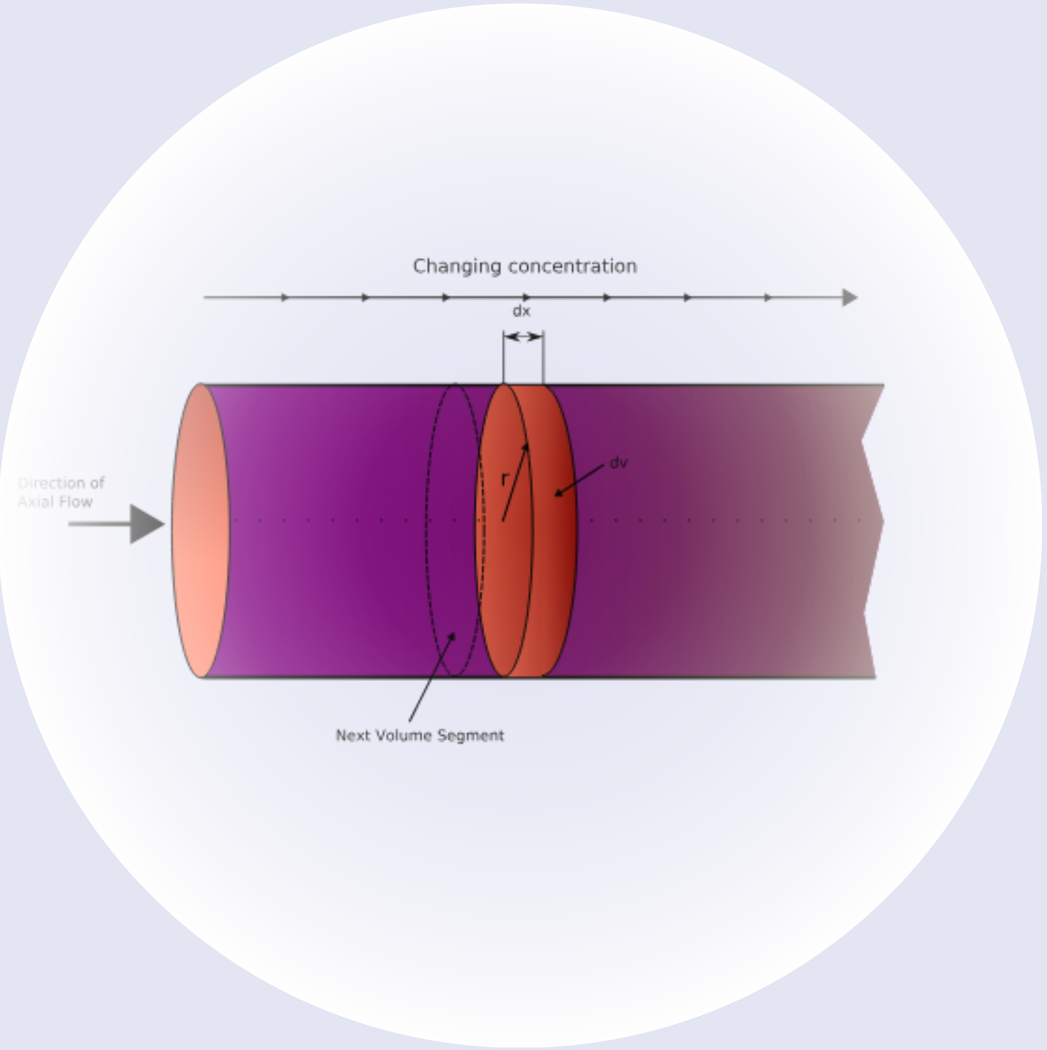
Chemical Reactor Volume Calculator

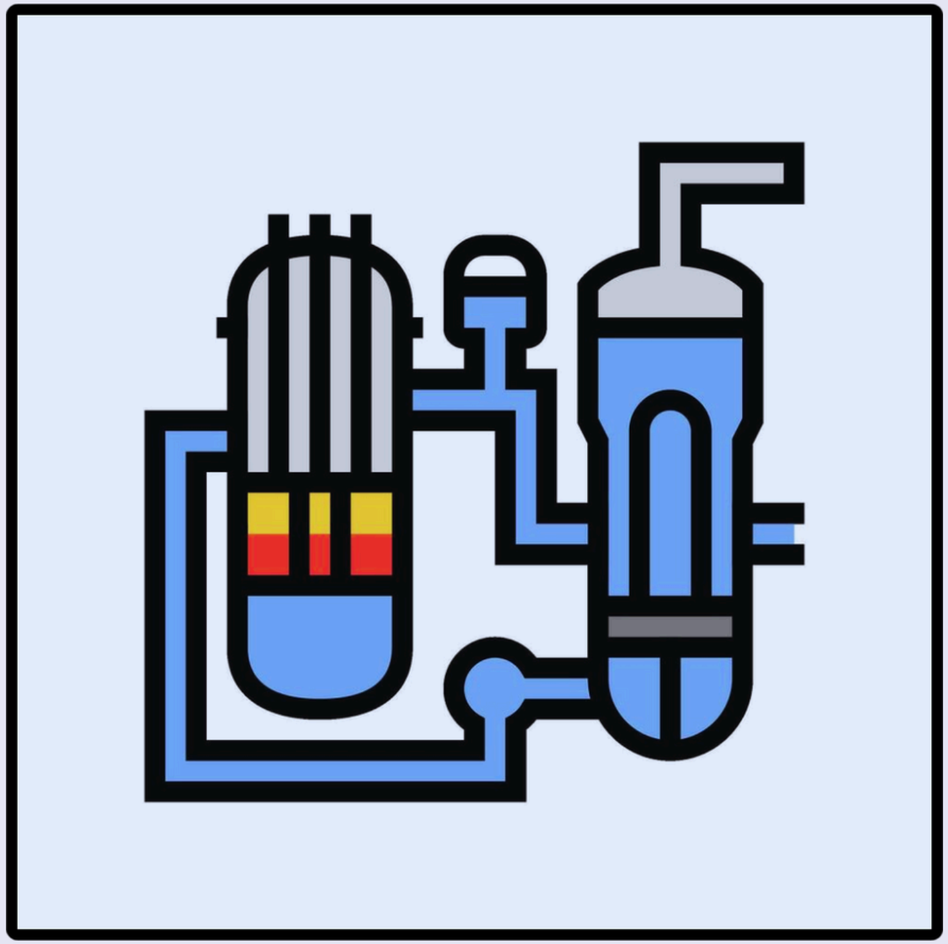
Ninad Gawade 2022CH71493
Varun Gawali 2022CH71505
Subham Singh 2022CH71512
Yogesh Yadav 2021CH10406



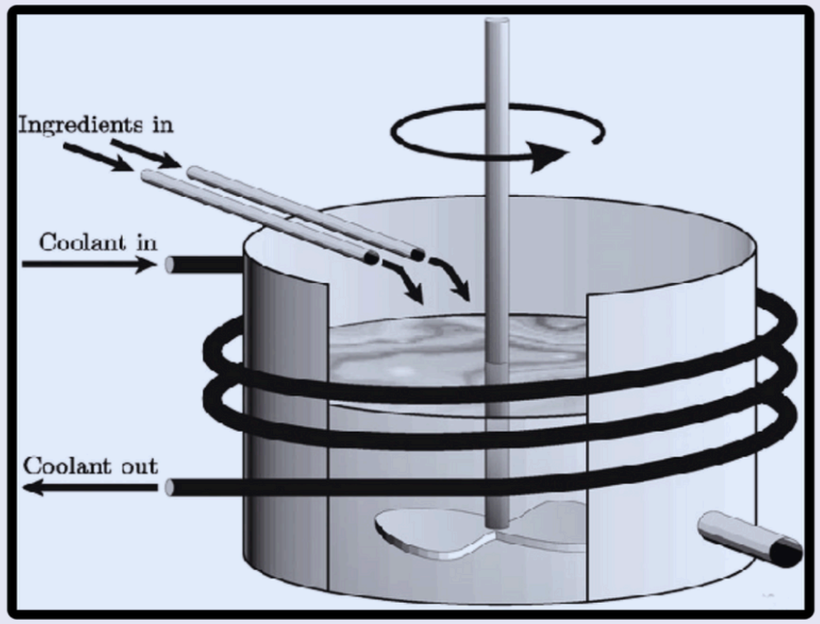
Aim

Our aim for this project is to calculate:

1. **PFR:**
   - **Rate of the reaction.**
   - **Volume of the reactor required.**
2. **CSTR:**
   - **Volume of the reactor required.**
   - **Mean Residence Time inside the reactor.**
3. **PBR:**
   - **Rate of the Reaction.**
   - **Weight of the Catalyst required.**
4. **Batch Reactor:**
   - **Time required for conversion.**



THEORY

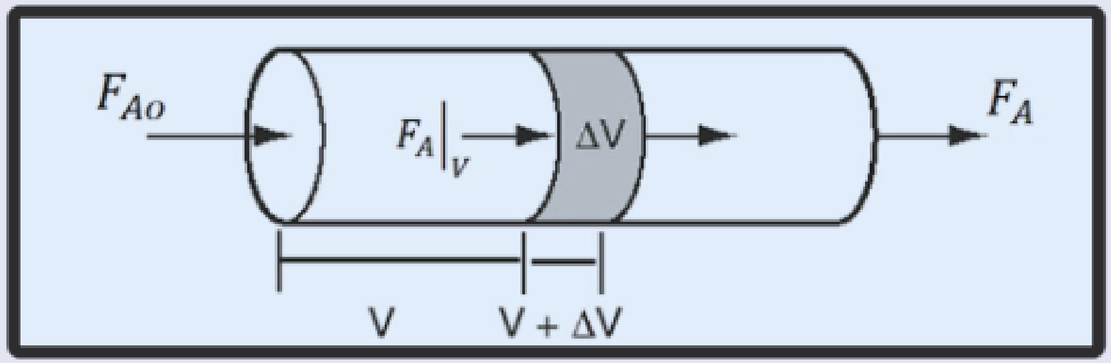


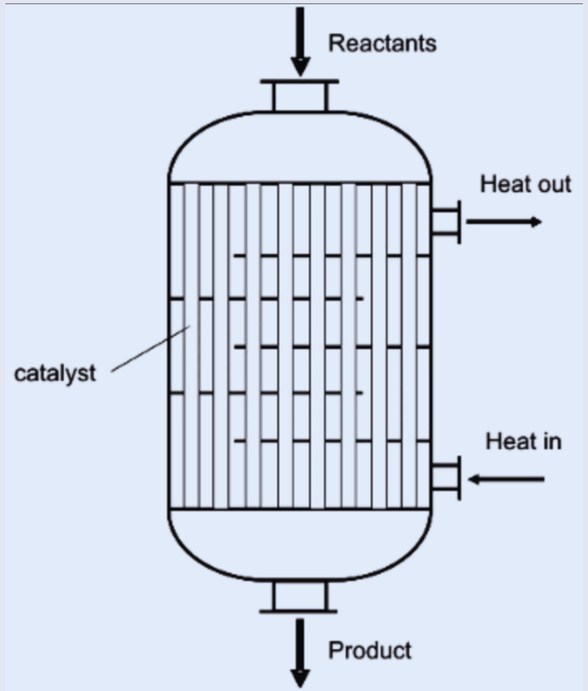
CSTR:

In a continuous stirred-tank reactor (CSTR), reactants are added continuously to a tank where they mix with the tank's contents, which are also continuously removed. The reaction progress is monitored and controlled by measuring the concentrations of reactants and products in the tank, and adjusting the flow rates accordingly.

PFR:

A plug flow reactor is a type of chemical reactor where a fluid flows through a pipe or tube and undergoes a chemical reaction while in transit. The reactants are introduced at one end of the reactor and flow through the reactor, undergoing conversion as they move through the reactor, and are removed at the other end.



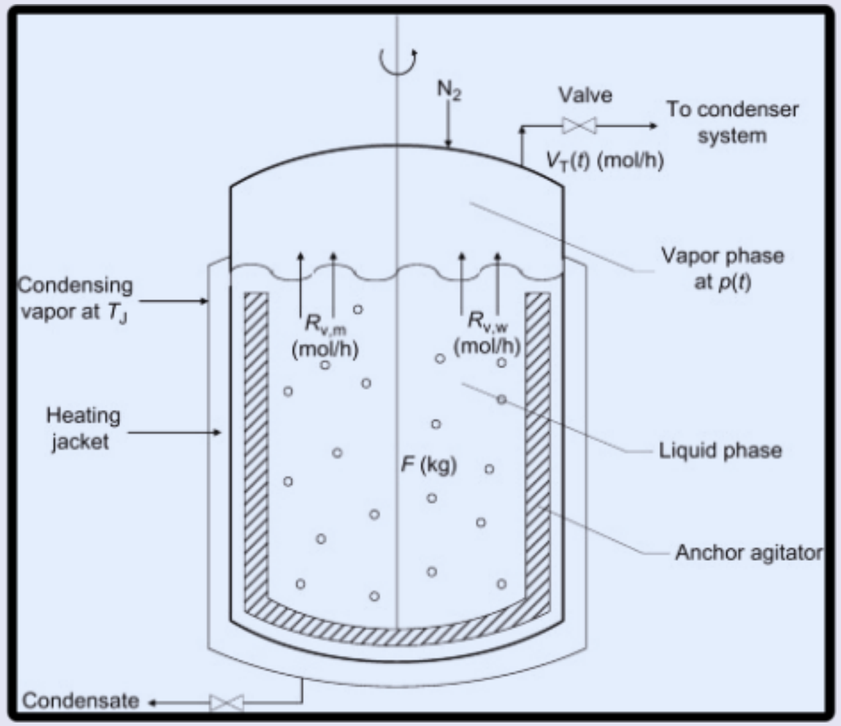


PBR:

Packed bed reactors are reactor vessels containing a fixed bed of catalytic material, they are widely used in the chemical process industry and find primary use in heterogeneous, gas-phase, catalytic reactions.

Batch Reactor:

A batch reactor is a chemical reactor in which a non-continuous reaction is conducted. They are used to study the behavior of fluids with materials under various conditions of temperature and pressure.



Formulas Used:

1. Solution algorithm

a. Mole balances (BR, CSTR, PFR, PBR):

$$N_{A0}\frac{dX}{dt} = -r_A V, \quad V = \frac{F_{A0}X}{-r_A}, \quad F_{A0}\frac{dX}{dV} = -r_A, \quad F_{A0}\frac{dX}{dW} = -r'_A$$

b. Rate law: For example,

$$-r'_A = kC_A^2$$

c. Stoichiometry:

$$A + \frac{b}{a}B \rightarrow \frac{c}{a}C + \frac{d}{a}D$$

(1) *Liquid phase:* $v = v_0$

$$C_A = C_{A0}(1-X)$$

(2) *Gas phase:* $v = v_0(1+\varepsilon X)\left(\frac{P_0}{P}\right)\left(\frac{T}{T_0}\right)$, where $\varepsilon = y_{A0}\delta = y_{A0}\left(\frac{d}{a}+\frac{c}{a}-\frac{b}{a}-1\right)$

$$p = \frac{P}{P_0}$$

$$f = v/v_0$$

$$C_A = \frac{F_A}{v} = \frac{F_{A0}(1-X)}{v} = \frac{F_{A0}(1-X)}{v_0(1+\varepsilon X)}\left(\frac{P}{P_0}\right)\frac{T_0}{T} = C_{A0}\left(\frac{1-X}{1+\varepsilon X}\right)p\,\frac{T_0}{T}$$

For a **PBR**

$$\frac{dp}{dW} = -\frac{\alpha(1+\varepsilon X)}{2p}\left(\frac{T}{T_0}\right)$$

$$\alpha = \frac{2\beta_0}{A_c(1-\phi)\rho_c P_0} \text{ and } \beta_0 = \frac{G(1-\phi)}{\rho_0 g_c D_p \phi^3}\left[\frac{150(1-\phi)\mu}{D_p} + 1.75G\right]$$

Variable density with $\varepsilon = 0$ or $\varepsilon X \ll 1$ and isothermal operation:

IFF ε = 0

$$p = \frac{P}{P_0} = (1-\alpha W)^{1/2}$$

Combining Equations (5-22) and (5-23) gives

$$\frac{dP}{dz} = -\underbrace{\frac{G(1-\phi)}{\rho_0 g_c D_p \phi^3}\left[\frac{150(1-\phi)\mu}{D_p} + 1.75G\right]}_{\beta_0}\frac{P_0}{P}\left(\frac{T}{T_0}\right)\frac{F_T}{F_{T0}}$$

Simplifying yields

$$\boxed{\frac{dP}{dz} = -\beta_0\frac{P_0}{P}\left(\frac{T}{T_0}\right)\frac{F_T}{F_{T0}}} \quad (5\text{-}24)$$

where β_0 is a constant that depends only on the properties of the packed bed (ϕ, D_p) and the fluid properties at the entrance conditions (i.e., μ, G, ρ_0, T_0, P_0). Typical units of β_0 are (atm/ft) or (Pa/m).

$$\boxed{\beta_0 = \frac{G(1-\phi)}{\rho_0 g_c D_p \phi^3}\left[\frac{150(1-\phi)\mu}{D_p} + 1.75G\right] \quad \left(\text{e.g., } \frac{\text{kPa}}{\text{m}}, \frac{\text{atm}}{\text{ft}}\right)} \quad (5\text{-}25)$$

For tubular packed-bed reactors, we are more interested in catalyst weight rather than the distance z down the reactor. The catalyst weight up to a distance of z down the reactor is

$$\overbrace{\left[\begin{matrix}\text{Weight of}\\ \text{catalyst}\end{matrix}\right]}^{W} = \overbrace{\left[\begin{matrix}\text{Volume of}\\ \text{solids}\end{matrix}\right]}^{(1-\phi)A_c z} \times \overbrace{\left[\begin{matrix}\text{Density of}\\ \text{solid catalyst}\end{matrix}\right]}^{\rho_c} \quad (5\text{-}26)$$

where A_c is the cross-sectional area. The *bulk density* of the catalyst, ρ_b (mass of catalyst per volume of reactor bed), is just the product of the density of the solid catalyst particles, ρ_c, and the fraction of solids, $(1-\phi)$:

Bulk density

$$\rho_b = \rho_c(1-\phi)$$

Using the relationship between z and W [Equation (5-26)], we can change our variables to express the Ergun equation in terms of catalyst weight:

Use this form for multiple reactions and membrane reactors.

$$\frac{dP}{dW} = -\frac{\beta_0}{A_c(1-\phi)\rho_c}\frac{P_0}{P}\left(\frac{T}{T_0}\right)\frac{F_T}{F_{T0}}$$

Further simplification yields

$$\frac{dP}{dW} = -\frac{\alpha}{2}\frac{T}{T_0}\frac{P_0}{P/P_0}\left(\frac{F_T}{F_{T0}}\right) \quad (5\text{-}27)$$

THANK YOU