BT209

Bioreaction Engineering

08/02/2023

Design of reactor

- So far we have considered the mathematical expression called the rate equation which describes the progress of a homogeneous reaction. The rate equation for a reacting component i is an intensive measure, and it tells how rapidly component i forms or disappears in a given environment as a function of the conditions there,

$$r_i = \frac{1}{V}\left(\frac{dN_i}{dt}\right)_{\text{by reaction}} = f(\text{conditions within the region of volume } V)$$

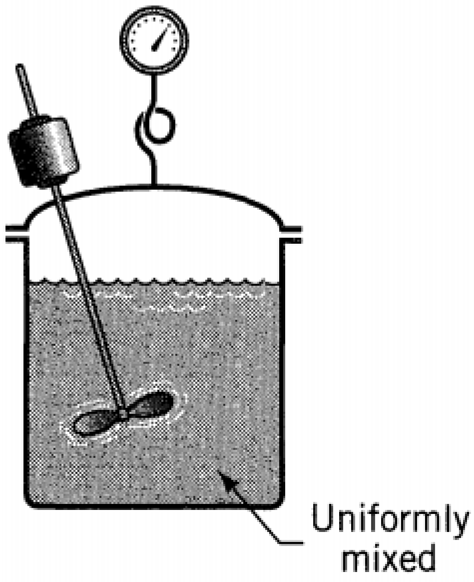
➢In reactor design we want to know **what size** and **type of reactor** and **method of operation** are **best for a given job**.

➢Because this **may require that the conditions in the reactor vary with position as well as time**, this question can only be answered by a proper integration of the rate equation for the operation.

➢This may pose **difficulties because the temperature and composition of the reacting fluid may vary from point to point within the reactor**, depending on the endothermic or exothermic character of the reaction, **the rate of heat addition or removal from the system**, and the **flow pattern of fluid through the vessel**.

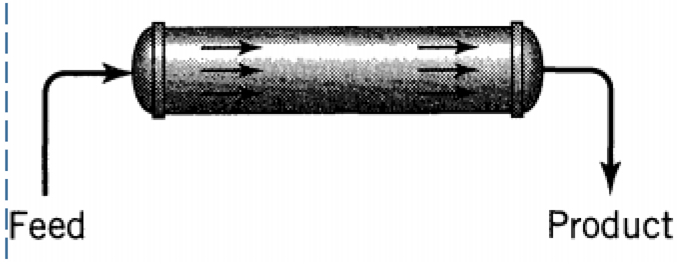
Cont..

Batch reactor (a)

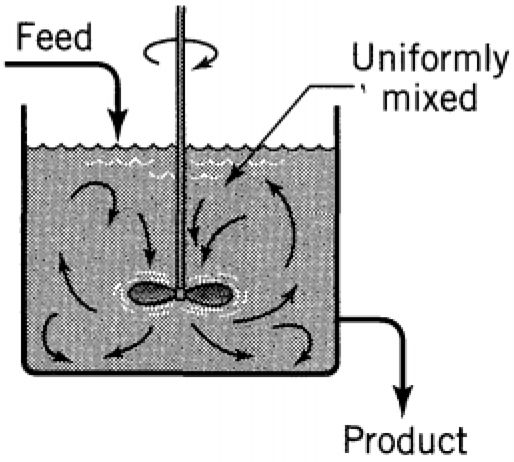


(a)

Flow reactor (b and c)

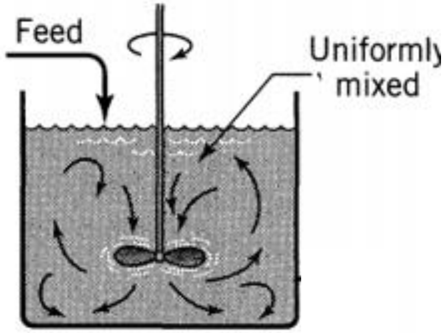


(b)



(c)

Semi batch (d)



- **Intermediate inlet**
- **No outlet**

(a) batch reactor,

(b) plug flow reactor, or PFR; and

(c) mixed flow reactor, or MFR
or Continuous stirred tank (CSTR)

- **No intermediate addition**

- **Continuous input and output**

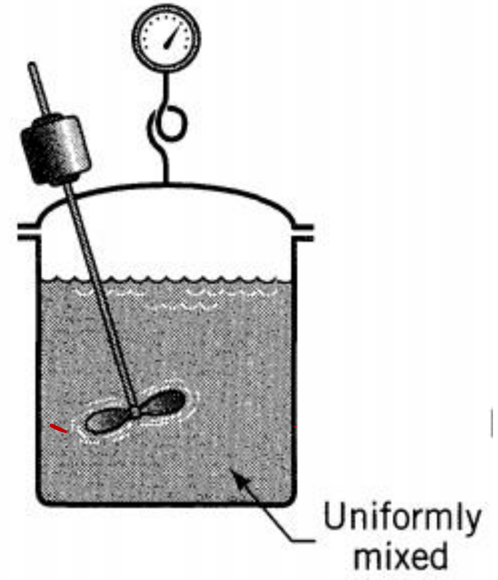
Ideal batch reactor

- In the batch reactor, the reactants are initially charged into a container, are well mixed, and are left to react for a certain period. The resultant mixture is then discharged.

- This is an unsteady-state operation where composition changes with time; however, at any instant the composition throughout the reactor is uniform (well mixed).

  ✓ The starting point for all design is the material balance expressed for any reactant (or product).

$$\begin{pmatrix}\text{rate of}\\ \text{reactant}\\ \text{flow into}\\ \text{element}\\ \text{of volume}\end{pmatrix} = \begin{pmatrix}\text{rate of}\\ \text{reactant}\\ \text{flow out}\\ \text{of element}\\ \text{of volume}\end{pmatrix} + \begin{pmatrix}\text{rate of reactant}\\ \text{loss due to}\\ \text{chemical reaction}\\ \text{within the element}\\ \text{of volume}\end{pmatrix} + \begin{pmatrix}\text{rate of}\\ \text{accumulation}\\ \text{of reactant}\\ \text{in element}\\ \text{of volume}\end{pmatrix}$$



Cont..

$$\begin{array}{c}\text{disappearance of A} \\ \text{by reaction,} \\ \text{moles/time}\end{array} = (-r_A)V = \left(\frac{\text{moles A reacting}}{(\text{time})(\text{volume of fluid})}\right)(\text{volume of fluid})$$

$$\begin{array}{c}\text{accumulation of A,} \\ \text{moles/time}\end{array} = \frac{dN_A}{dt} = \frac{d[N_{A0}(1-X_A)]}{dt} = -N_{A0}\frac{dX_A}{dt}$$

$$\boxed{(-r_A)V = N_{A0}\frac{dX_A}{dt}}$$

Rearranging and integrating then gives

$$t = N_{A0}\int_0^{X_A}\frac{dX_A}{(-r_A)V}$$ ⟸ **(Design equation of batch reactor)**

- This is the general equation showing the time required to achieve a conversion X_A for either isothermal or nonisothermal operation.
- The volume of reacting fluid and the reaction rate remain under the integral sign, for in general they both change as reaction proceeds.

Cont..

This equation may be simplified for a number of situations. **If the density of the fluid remains constant (constant volume system)**, we obtain

$$t = C_{A0} \int_0^{X_A} \frac{dX_A}{-r_A} = - \int_{C_{A0}}^{C_A} \frac{dC_A}{-r_A} \qquad \text{for } \varepsilon_A = 0$$

For all reactions in which the **volume of reacting mixture changes proportionately with conversion**, such as in single gas-phase reactions with significant density changes

$$t = N_{A0} \int_0^{X_A} \frac{dX_A}{(-r_A)V_0(1+\varepsilon_A X_A)} = C_{A0} \int_0^{X_A} \frac{dX_A}{(-r_A)(1+\varepsilon_A X_A)}$$

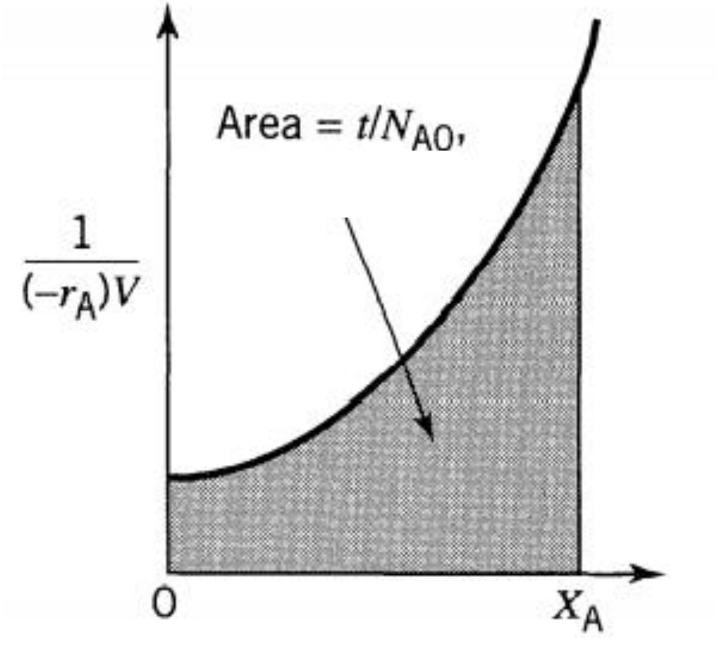
- They are applicable to both isothermal and nonisothermal operations. For the latter the variation of rate with temperature, and the variation of temperature with conversion, must be known before solution is possible.

Graphical representation of the performance equations for batch reactor

$$t = N_{A0}\int_0^{X_A} \frac{dX_A}{(-r_A)V}$$

$$t = C_{A0}\int_0^{X_A}\frac{dX_A}{-r_A} = -\int_{C_{A0}}^{C_A}\frac{dC_A}{-r_A} \qquad \text{for } \varepsilon_A = 0$$

General case



Constant-density systems only