BT209

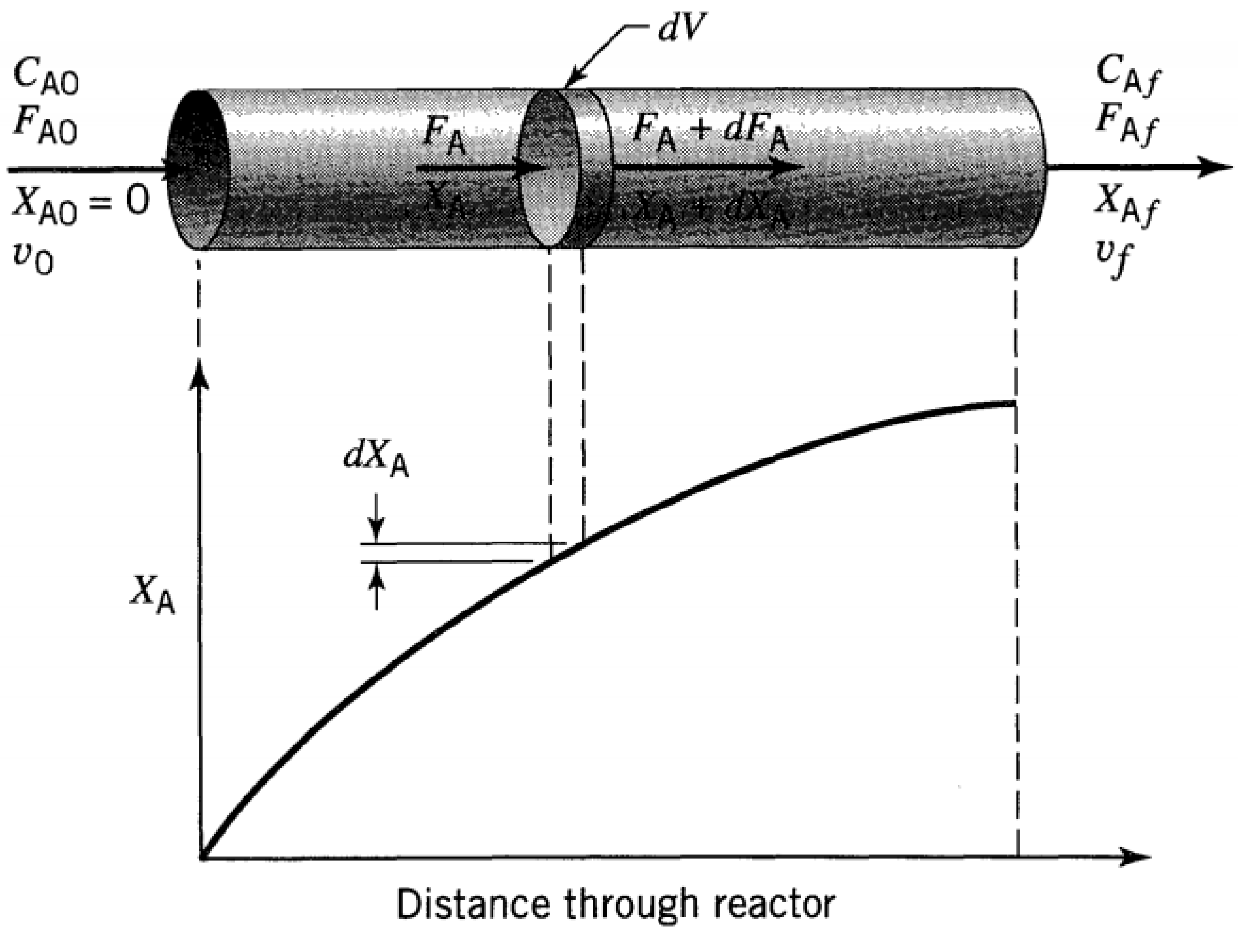
Bioreaction Engineering

15/02/2023

Steady sate Plug flow reactor (PFR)

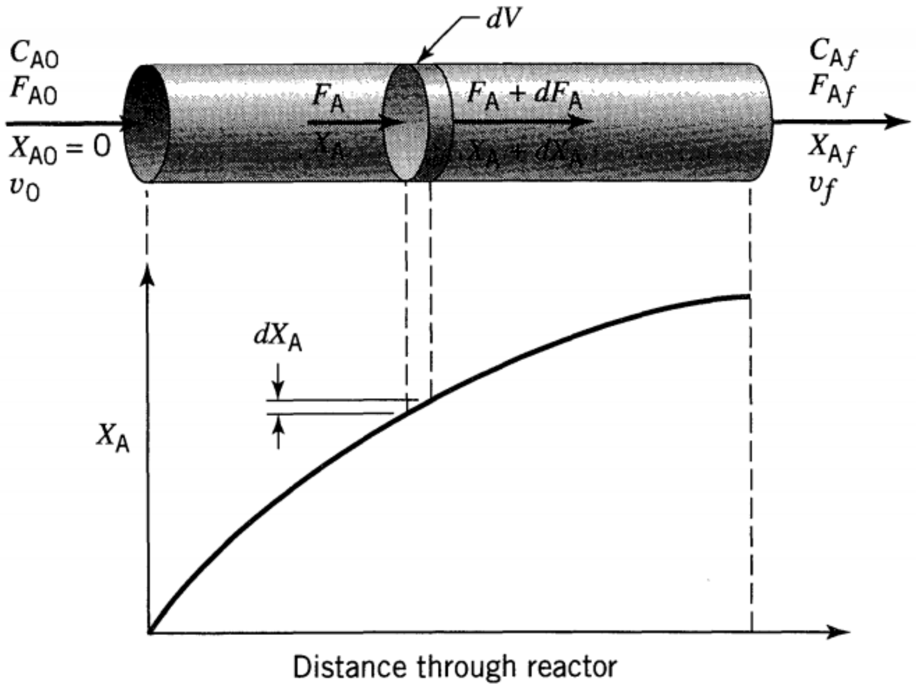
- **Pattern of flow as plug flow.**
  - It is characterized by the fact that the flow of fluid through the reactor is orderly with no element of fluid overtaking or mixing with any other element ahead or behind.
  - Actually, there may be lateral mixing of fluid in a plug flow reactor; however, there must be no mixing or diffusion along the flow path

- In a plug flow reactor the composition of the fluid varies from point to point along a flow path;



Cont.

➢**Material balance** for a reaction component must be made for a differential element of volume d*V*.



❑ **For reactant A**

<u>**For volume d*V***</u>

$$\text{input} = \text{output} + \text{disappearance by reaction} + \underbrace{\cancel{\text{accumulation}}}_{=0}$$

$$\text{input of A, moles/time} = F_A$$

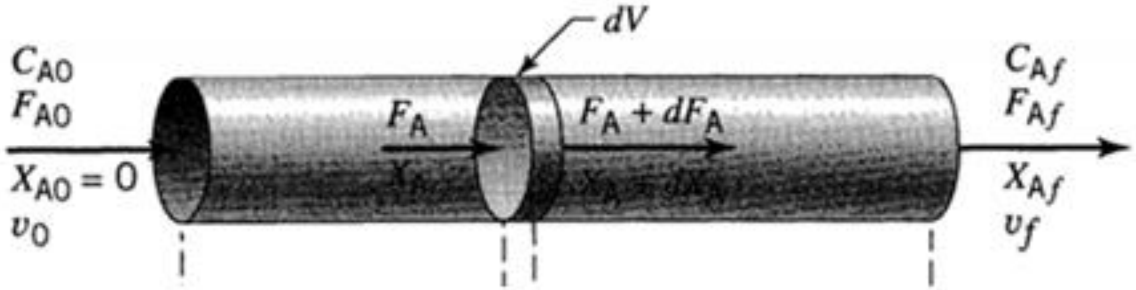
$$\text{output of A, moles/time} = F_A + dF_A$$

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

$$F_A = (F_A + dF_A) + (-r_A)dV$$

Cont.

Noting that



$$dF_A = d[F_{A0}(1 - X_A)] = -F_{A0}dX_A$$

$$\boxed{F_{A0}dX_A = (-r_A)dV}$$

➢This, then, is the equation which accounts for A in the differential section of reactor of volume dV.

➢ For the reactor as a whole the expression must be integrated. Now F_{A0}, the feed molar flow rate, is constant, but r_A is certainly dependent on the concentration or conversion of materials.

$$\int_0^V \frac{dV}{F_{A0}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A}$$

Cont.

Thus

or

$$\boxed{\begin{aligned} \frac{V}{F_{A0}} &= \frac{\tau}{C_{A0}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A} \\ \tau = \frac{V}{v_0} &= \frac{VC_{A0}}{F_{A0}} = C_{A0}\int_0^{X_{Af}} \frac{dX_A}{-r_A} \end{aligned}} \qquad \text{any } \varepsilon_A$$

- Equation allows the determination of reactor size for a given feed rate and required conversion

As a more general expression for plug flow reactors, if the feed on which conversion is based, subscript 0, enters the reactor partially converted, subscript i, and leaves at a conversion designated by subscript f, we have

$$\frac{V}{F_{A0}} = \int_{X_{Ai}}^{X_{Af}} \frac{dX_A}{-r_A}$$

Special case: constant volume

For the special case of *constant-density systems*

$$X_A = 1 - \frac{C_A}{C_{A0}} \quad \text{and} \quad dX_A = -\frac{dC_A}{C_{A0}}$$

$$\boxed{\begin{aligned} \frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} &= \int_0^{X_{Af}} \frac{dX_A}{-r_A} = -\frac{1}{C_{A0}} \int_{C_{A0}}^{C_{Af}} \frac{dC_A}{-r_A} \\ \tau = \frac{V}{v_0} &= C_{A0} \int_0^{X_{Af}} \frac{dX_A}{-r_A} = -\int_{C_{A0}}^{C_{Af}} \frac{dC_A}{-r_A} \end{aligned}}$$

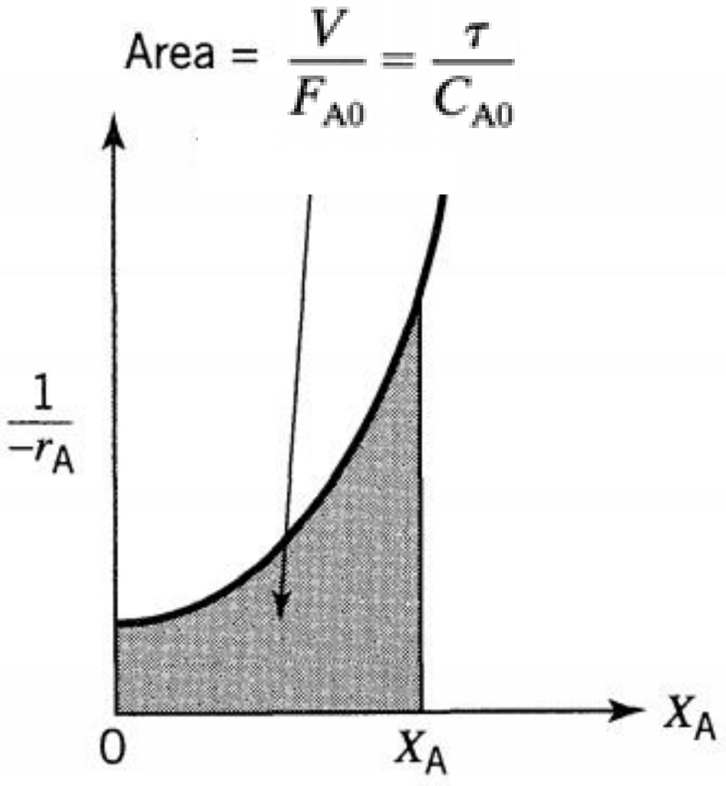
$$\varepsilon_A = 0$$

Graphical representation

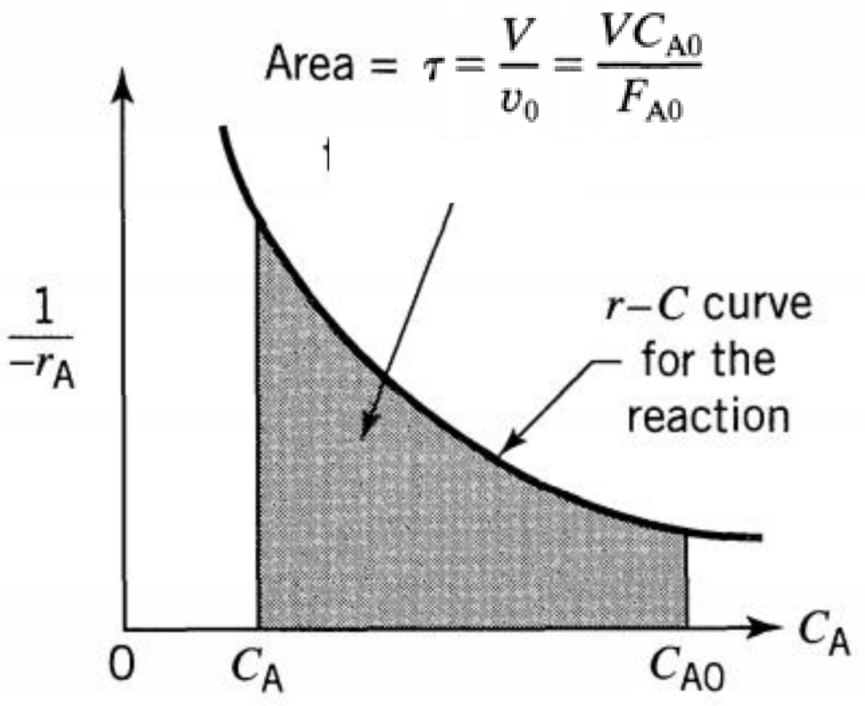
$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A}$$

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A} = -\frac{1}{C_{A0}} \int_{C_{A0}}^{C_{Af}} \frac{dC_A}{-r_A}$$

General case



Constant-density systems only



For zero order and first order

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A}$$

Zero-order homogeneous reaction, any constant ε_A

$$k\tau = \frac{kC_{A0}V}{F_{A0}} = C_{A0}X_A$$

First-order irreversible reaction, A → products, any constant ε_A,

$$\boxed{k\tau = -(1+\varepsilon_A)\ln(1-X_A) - \varepsilon_A X_A}$$

For 2nd order

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A}$$

Second-order irreversible reaction, A + B → products with equimolar feed or 2A → products, any constant ε_A,

$$C_{A0}k\tau = 2\varepsilon_A(1+\varepsilon_A)\ln(1-X_A) + \varepsilon_A^2 X_A + (\varepsilon_A+1)^2 \frac{X_A}{1-X_A}$$

Compare batch, CSTR and PFR

In general

Batch

$$t = C_{A0} \int_0^{X_A} \frac{dX_A}{-r_A}$$

PFR

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A}$$

CSTR

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}}$$

For constant density, for $\varepsilon_A = 0$

Batch

$$t = C_{A0} \int_0^{X_A} \frac{dX_A}{-r_A} = -\int_{C_{A0}}^{C_A} \frac{dC_A}{-r_A}$$

PFR

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A} = -\frac{1}{C_{A0}} \int_{C_{A0}}^{C_{Af}} \frac{dC_A}{-r_A}$$

CSTR

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \frac{X_A}{-r_A} = \frac{C_{A0} - C_A}{C_{A0}(-r_A)}$$

For *systems of constant density* (constant-volume batch and constant-density plug flow) the performance equations are identical, τ for plug flow is equivalent to t for the batch reactor, and the equations can be used interchangeably.

Problem 1

A specific enzyme acts as catalyst in the fermentation of reactant A. At a given enzyme concentration in the aqueous feed stream (25 litre/min) find the volume of plug flow reactor needed for 95% conversion of reactant A (CA0 = 2 mol / liter). The kinetics of the fermentation at this enzyme concentration is given by

A → R

$$-r_A = \frac{0.1C_A}{1+0.5C_A}\frac{mol}{liter.min}$$

Solution:

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A} = -\frac{1}{C_{A0}}\int_{C_{A0}}^{C_{Af}} \frac{dC_A}{-r_A}$$

$$k_1\frac{V}{v} = ln\frac{C_{A0}}{C_A} + k_2(C_{A0} - C_A)$$

$k_1 = 0.1$, $k_2 = 0.5$, $C_{A0} = 2$ mol/lt, $v = 25$ lt/min, $C_A = 0.1$ mol/lt

$V = 986$ lt ~ 1 m^3

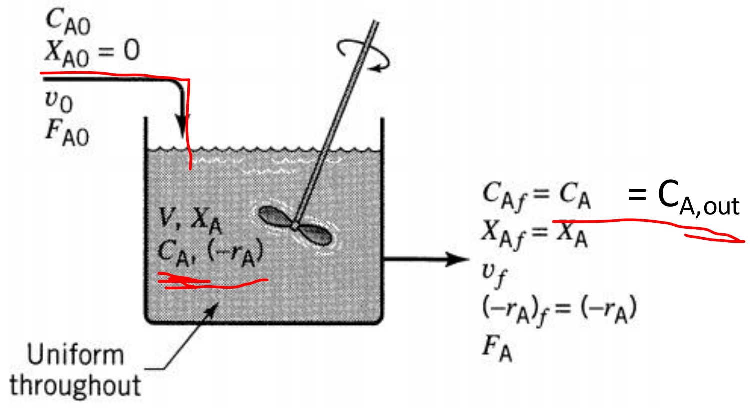
Problem 2

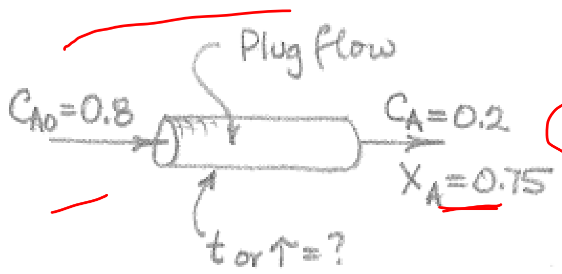
The aqueous decomposition of A is studied in an experimental mixed flow reactor. The results in Table are obtained in steady-state runs. To obtain 75% conversion of reactant in a feed, C_{A0} = 0.8 mol/liter, what holding time is needed in a plug flow reactor?

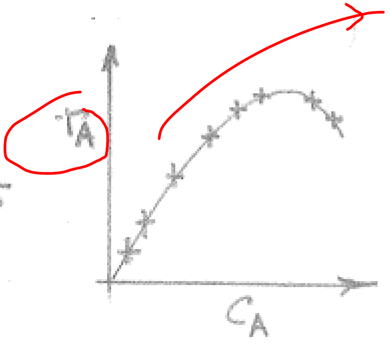
Concentration of A, mol/liter		Holding Time, sec
In Feed	In Exit Stream	
2.00	0.65	300
2.00	0.92	240
2.00	1.00	250
1.00	0.56	110
1.00	0.37	360
0.48	0.42	24
0.48	0.28	200
0.48	0.20	560

Solution: Problem 2

τ sec	C_{A0}	$C_{A,out}$	$-\frac{1}{r_A} = \frac{\tau}{C_{A0}-C_{A,out}}$ ... at $C_{A,out}$
300	2	0.65	300/(2-0.65) = 222
240	2	0.92	222
250	2	1.00	250
110	1	0.56	250
360	1	0.37	572
24	0.48	0.42	400
200	0.48	0.28	1000
560	0.48	0.20	2000

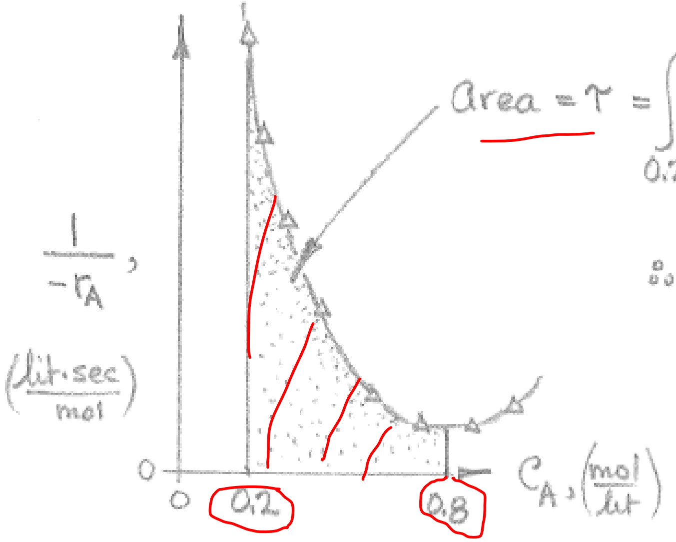






$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A} = -\frac{1}{C_{A0}} \int_{C_{A0}}^{C_{Af}} \frac{dC_A}{-r_A}$$

$\varepsilon_A = 0$



Area = $\tau = \int_{0.2}^{0.8} \frac{dC_A}{-r_A}$ = 300 sec

∴ for a plug flow reactor

τ = t = 300 sec