BT209

Bioreaction Engineering

22/03/2023

Autocatalytic reaction and reactor

n^{th} order reaction (n>0) A→R $-r_A = -\frac{dC_A}{dt} = kC_A^n$

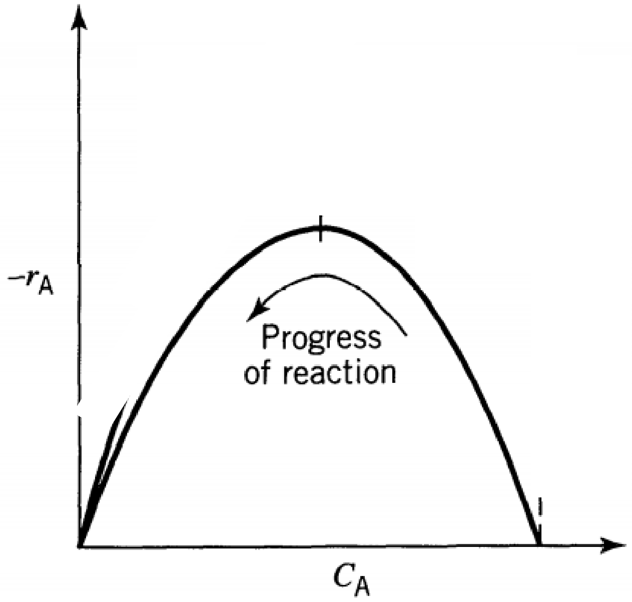
When a material reacts away (A→R) by any n^{th} order rate (n > 0) in a batch reactor,

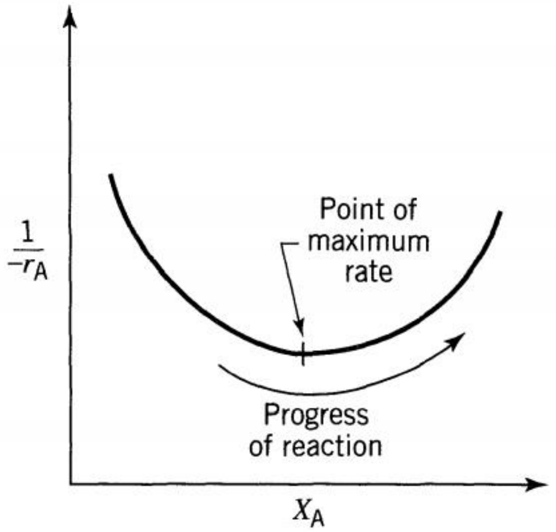
- its rate of disappearance is rapid at the start when the concentration of reactant is high.
- This rate then slows progressively as reactant is consumed.

Autocatalytic reaction

$$A + R \rightarrow R + R, \qquad -r_A = kC_A^a C_R^r$$

- The rate at the start is low because little product is present;
- it increases to a maximum as product is formed
- then drops again to a low value as reactant is consumed.

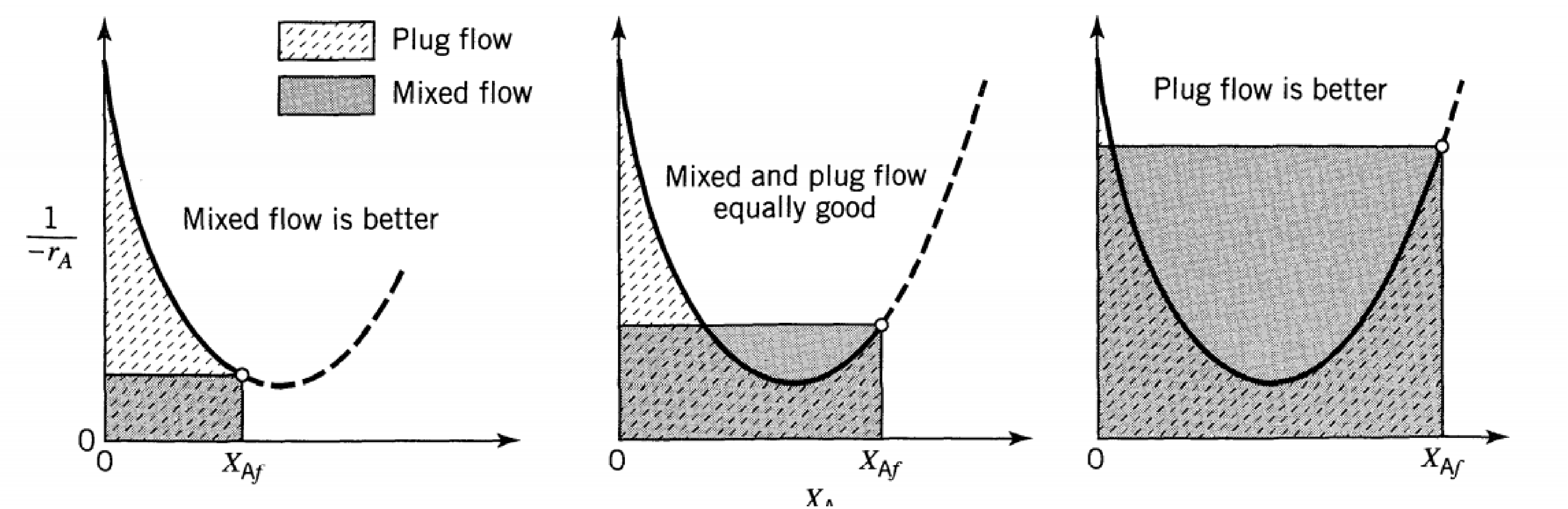




PFR Vs CSTR for autocatalytic reaction

For any particular rate-concentration curve a comparison of areas in Fig. shows which reactor is superior (which requires a smaller volume) for a given job.

1. At low conversion the mixed reactor is superior to the plug flow reactor.
2. At high enough conversions the plug flow reactor is superior.

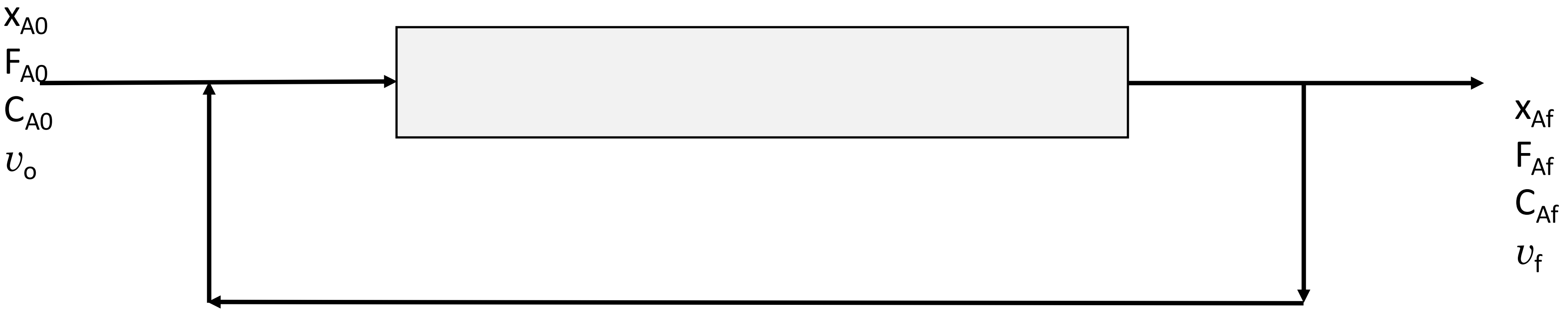


- ➢ These findings differ from ordinary nth-order reactions (n > 0) where the plug flow reactor is always more efficient than the mixed flow reactor.

Optimum Recycle Operations

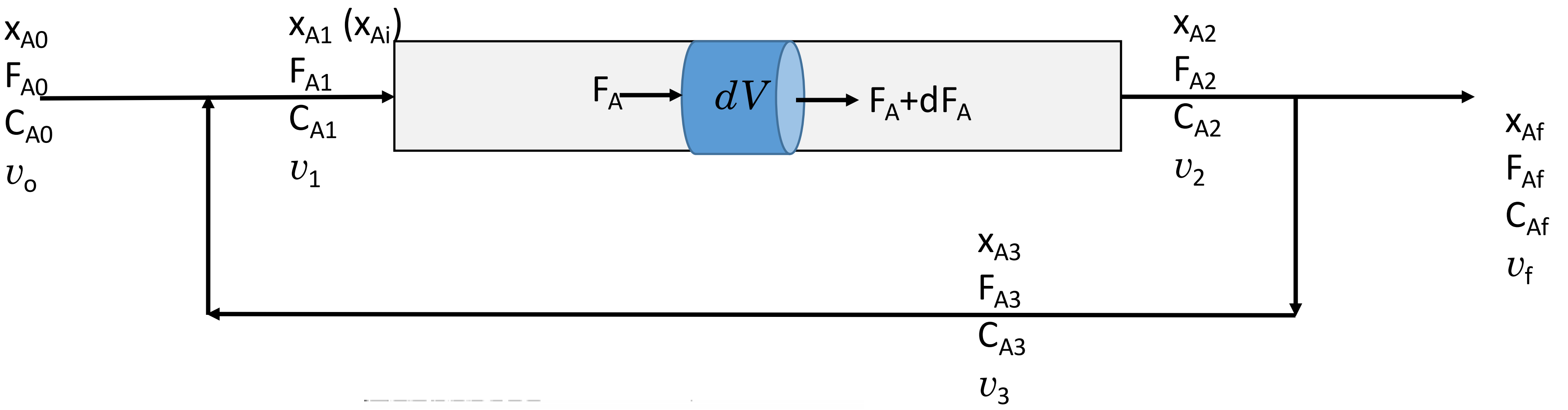
- In addition, we should note that a plug flow reactor will not operate at all with a feed of pure reactant. In such a situation the feed must be continually primed with product, an ideal opportunity for using a recycle reactor.

- Using optimization problems we can find the optimum recycle ratio which gives the minimum reactor volume or minimum space time



$$\boldsymbol{R} = \frac{\text{volume of fluid returned to the reactor entrance}}{\text{volume leaving the system}}$$

Cont.



$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = (\boldsymbol{R}+1)\int_{\left(\frac{\boldsymbol{R}}{\boldsymbol{R}+1}\right)X_{Af}}^{X_{Af}} \frac{dX_A}{-r_A}$$

✓The optimum recycle ratio is found by differentiating Eq. with respect to R and setting to zero, thus

$$\frac{d(\tau/C_{A0})}{d\boldsymbol{R}} = 0$$

$$\frac{d(V/F_{A0})}{dR} = 0$$

Cont.

$$\frac{d(\tau/C_{A0})}{d\boldsymbol{R}} = 0$$ for $$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = (\boldsymbol{R}+1)\int_{X_{Ai}=\left(\frac{\boldsymbol{R}}{\boldsymbol{R}+1}\right)X_{Af}}^{X_{Af}} \frac{dX_A}{-r_A}$$

$$F(\boldsymbol{R}) = \int_{a(\boldsymbol{R})}^{b(\boldsymbol{R})} f(x,\boldsymbol{R})\,dx$$

$$\frac{dF}{d\boldsymbol{R}} = \int_{a(\boldsymbol{R})}^{b(\boldsymbol{R})} \frac{\partial f(x,\boldsymbol{R})}{\partial \boldsymbol{R}}\,dx + f(\mathrm{b},\boldsymbol{R})\frac{db}{d\boldsymbol{R}} - f(a,\boldsymbol{R})\frac{da}{d\boldsymbol{R}}$$

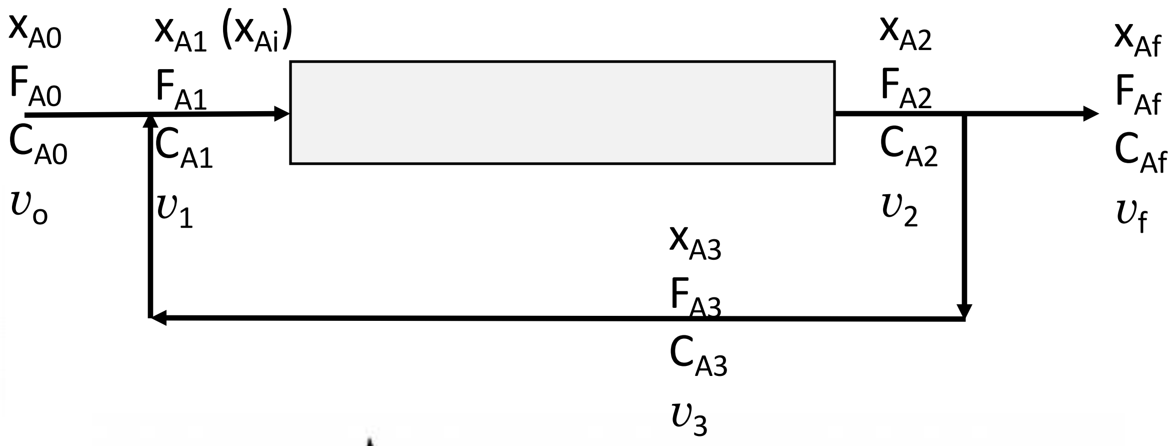
$$\frac{d(\tau/C_{A0})}{d\boldsymbol{R}} = 0 = \int_{X_{Ai}}^{X_{Af}} \frac{dX_A}{(-r_A)} + 0 - \left.\frac{\boldsymbol{R}+1}{(-r_A)}\right|_{X_{Ai}} \frac{dX_{Ai}}{d\boldsymbol{R}}$$

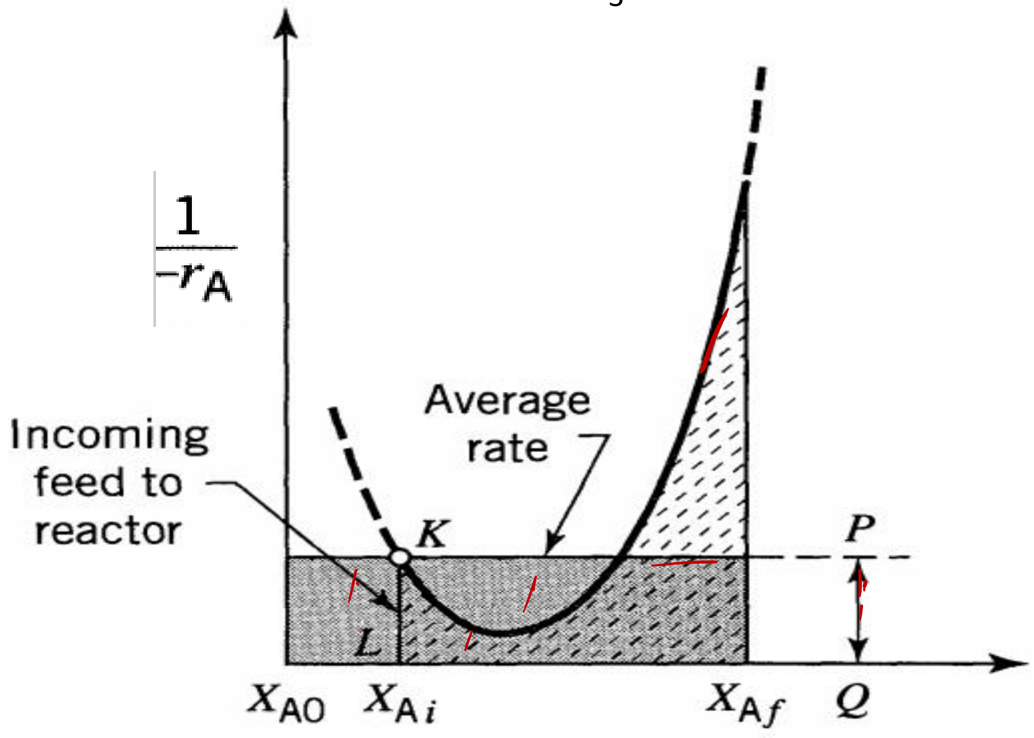
Cont.

$$X_{Ai} = \left(\frac{R}{R+1}\right) X_{Af} \quad \Rightarrow \quad \frac{dX_{Ai}}{dR} = \frac{X_{Af}}{(R+1)^2}$$

$$\frac{d(\tau/C_{A0})}{dR} = 0 = \int_{X_{Ai}}^{X_{Af}} \frac{dX_A}{(-r_A)} + 0 - \frac{R+1}{(-r_A)}\bigg|_{X_{Ai}} \frac{dX_{Ai}}{dR}$$

$$\boxed{\frac{1}{-r_A}\bigg|_{X_{Ai}} = \frac{\int_{X_{Ai}}^{X_{Af}} \frac{dX_A}{-r_A}}{(X_{Af} - X_{Ai})}}$$

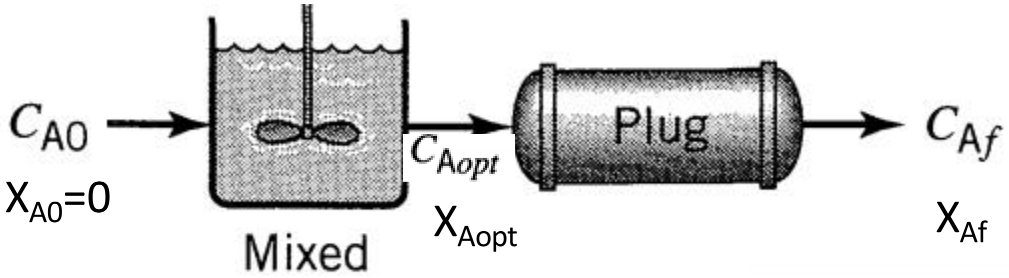


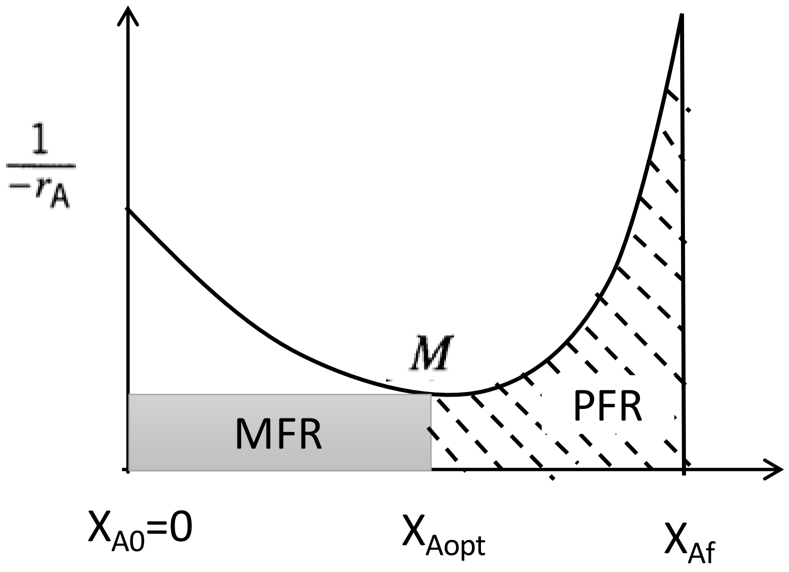


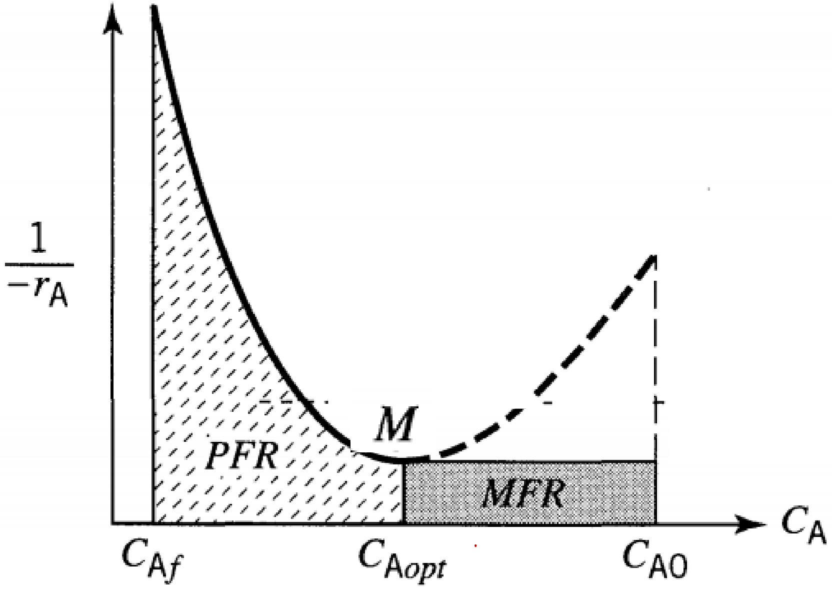
✓**In words, the optimum recycle ratio introduces to the reactor a feed whose 1/(-r_A) value (KL in Fig.) equals the average 1/(-r_A) value in the reactor as a whole (PQ in Fig.).**

Reactor combination for autocatalytic reaction without recycle

- For autocatalytic reactions
  - In general, for a rate-concentration curve as shown in Fig one should always try to reach point M in one step (using mixed flow in a single reactor), then follow with plug flow or as close to plug flow as possible. This procedure is shown as the shaded area in Fig.







Occurrence of Autocatalytic Reactions

- The most important examples of autocatalytic reactions are the broad class of fermentation reactions which result from the reaction of microorganism on an organic feed.

- When they can be treated as single reactions, the methods of this chapter can be applied directly.

$$S + \text{Cell} \rightarrow \text{More cell}$$