CHEN 416: CHEMICAL REACTION ENGINEERING II

DESIGNS FOR SINGLE REACTIONS AND SIZE COMPARISON FOR SINGLE REACTORS.

LEARNING OBJECTIVES

- At the end of this week's lecture, students should be able to:
  - Differentiate between holding time and space time.
  - Design and compare MFR and PFRs for single reactions
  - Design multiple reactors for single reaction
    - Multiple reactors in series
    - Multiple reactors in parallel

HOLDING TIME AND SPACE-TIME FOR FLOW REACTORS

- The distinction between these two measures of time, τ and $\bar{t}$ is as shown from their definitions. They are defined as follows:
- Space-time:

$$\tau = \begin{pmatrix} \text{time needed to} \\ \text{treat one reactor} \\ \text{volume of feed} \end{pmatrix} = \frac{V}{v_0} = \frac{C_{A0}V}{F_{A0}}, \quad [\text{hr}]$$

- Holding time:

$$\bar{t} = \begin{pmatrix} \text{mean residence time} \\ \text{of flowing material} \\ \text{in the reactor} \end{pmatrix}$$

$$= C_{A0}\int_0^{X_A} \frac{dX_A}{(-r_A)(1+\varepsilon_A X_A)}, \quad [\text{hr}]$$

- For constant density systems (all liquids and constant density gases)

$$\tau = \bar{t} = \frac{V}{v}$$

- For changing density systems $\tau \neq \bar{t}$ and $\bar{t} \neq V/v_0$, in which case it becomes difficult to find how these terms are related.

HOLDING TIME AND SPACE-TIME FOR FLOW REACTORS

- The value of τ depends on what happens in the reactor, while the value of $\bar{t}$ is independent of what happens in the reactor.
- Holding time $\bar{t}$ does not appear in the performance equations developed for flow systems, while it is seen that space-time τ or V/F_{A0} does naturally appear.
- Hence, τ or V/F_{A0} is the proper performance measure for flow systems.

DESIGN FOR SINGLE REACTIONS

- In chemical reaction, there are many ways of processing a fluid:
  - in a single batch or flow reactor,
  - in a chain of reactors possibly with inter-stage feed injection or heating,
  - in a reactor with recycle of the product stream using various feed ratios and conditions, and so on.
- Which scheme should we use?
- Factors to be considered in answering this question; for example,
  - the reaction type,
  - planned scale of production,
  - cost of equipment and operations,
  - safety,
  - stability and flexibility of operation,
  - equipment life expectancy,
  - length of time that the product is expected to be manufactured,
  - ease of convertibility of the equipment to modified operating conditions or to new and different processes.

DESIGN FOR SINGLE REACTIONS

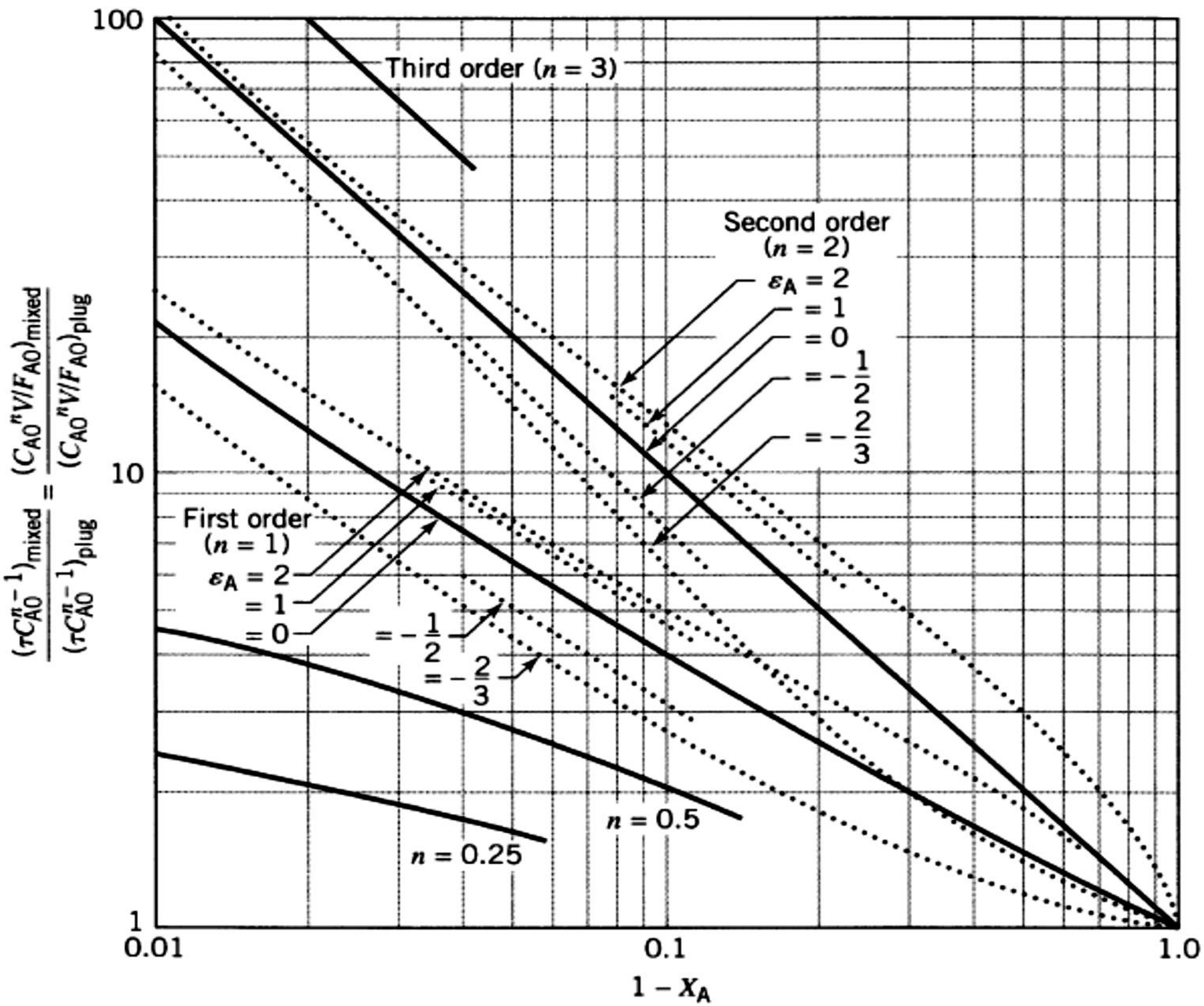
- For good design, all these factors are subjected to experience, engineering judgment, and a sound knowledge of the characteristics of the various reactor systems, the choice will also be dictated by the economics of the overall process.
- The reactor system selected will influence the economics of the process by dictating the size of the units needed and fixing the ratio of products formed.
- The first factor, reactor size, may well vary a hundredfold among competing designs while the second factor, product distribution, is usually of prime consideration where it can be varied and controlled.
- In *single reactions;* the reaction progress is described and followed adequately by using one and only one rate expression coupled with the necessary stoichiometric and equilibrium expressions (synonymous to elementary reactions).
- For such reactions product distribution is fixed; hence, the important factor in comparing designs is the reactor size.

SIZE COMPARISON OF SINGLE REACTORS

- **MFR Versus PFR**
- For a given duty the ratio of sizes of MFRs and PFRs will depend on the extent of reaction, the stoichiometry, and the form of the rate equation.
- For n[th] order rate law $$-r_A = -\frac{1}{V}\frac{dN_A}{dt} = kC_A^n$$
  - where n varies anywhere from zero to three.
- For MFR the performance Eq. for n[th] order rate law is given
- $$\tau_m = \left(\frac{C_{A0}V}{F_{A0}}\right)_m = \frac{C_{A0}X_A}{-r_A} = \frac{1}{kC_{A0}^{n-1}}\frac{X_A(1+\varepsilon_A X_A)^n}{(1-X_A)^n} \qquad 4\text{-}1$$
- whereas for PFR, the performance equation for nth order rate law is given as
- $$\tau_p = \left(\frac{C_{A0}V}{F_{A0}}\right)_p = C_{A0}\int_0^{X_A}\frac{dX_A}{-r_A} = \frac{1}{kC_{A0}^{n-1}}\int_0^{X_A}\frac{(1+\varepsilon_A X_A)^n dX_A}{(1-X_A)^n} \qquad 4\text{-}2$$
- Dividing 4-1 by 4-2, it yields

DESIGN FOR SINGLE REACTIONS

- $$\frac{(\tau C_{A0}^{n-1})_m}{(\tau C_{A0}^{n-1})_p} = \frac{\left(\frac{C_{A0}^n V}{F_{A0}}\right)_m}{\left(\frac{C_{A0}^n V}{F_{A0}}\right)_p} = \frac{\left[X_A\left(\frac{1+\varepsilon_A X_A}{1-X_A}\right)^n\right]_m}{\left[\int_0^{X_A}\left(\frac{1+\varepsilon_A X_A}{1-X_A}\right)^n dX_A\right]_p} \qquad \text{4-3}$$
- With constant density, or $\varepsilon = 0$, this expression integrates to
- $$\frac{(\tau C_{A0}^{n-1})_m}{(\tau C_{A0}^{n-1})_p} = \frac{\left[\frac{X_A}{(1-X_A)^n}\right]_m}{\left[\frac{(1-X_A)^{1-n}-1}{n-1}\right]_p}, \qquad n \neq 1 \qquad \text{4-4a}$$
- or
- $$\frac{(\tau C_{A0}^{n-1})_m}{(\tau C_{A0}^{n-1})_p} = \frac{\left(\frac{X_A}{1-X_A}\right)_m}{-\ln(1-X_A)_p}, \qquad n = 1 \qquad \text{4-4b}$$
- Equations 4-2 and 4-4a and b can be displayed in graphical form to provide a quick comparison of the performance of plug flow with mixed flow reactors.



- The ordinate becomes the volume ratio V_m/V_p or space-time ratio τ_m/τ_p if the same quantities of identical feed are used.

Fig.4-1Comparison of performance of single MFRs and PFRs for the n[th] order rxns

DESIGN FOR SINGLE REACTIONS

- For identical C_{A0} and F_{A0}, the ordinate of the graph gives directly the volume ratio required for any specified conversion.
- Figure 4-1 shows the following.
  - For any particular duty and for all positive reaction orders the MFR is always larger than the PFR. The ratio of volumes increases with reaction order.
  - When conversion is small, the reactor performance is only slightly affected by flow type. The performance ratio increases very rapidly at high conversion; consequently, a proper representation of the flow becomes very important in this range of conversion.
  - Density variation during reaction affects design; however, it is normally of secondary importance compared to the difference in flow type.

DESIGN FOR SINGLE REACTIONS

- For variation of reactant ratio for Second-order reactions of two components and of the type

$$A + B \rightarrow \text{products}, \qquad M = C_{B0}/C_{A0}$$

$$-r_A = -r_B = kC_AC_B$$

- behave as second-order reactions of one component when the reactant ratio is unity. Thus

$$-r_A = kC_AC_B = kC_A^2 \qquad \text{when } M = 1$$

- On the other hand, when a large excess of reactant B is used then its concentration does not change appreciably $(C_B = C_{B0})$ and the reaction approaches first-order behavior with respect to the limiting component **A,** or

$$-r_A = kC_AC_B = (kC_{B0})C_A = k'C_A \qquad \text{when } M \gg 1$$

- Thus in Fig. 4-1, and in terms of the limiting component A, the size ratio of MFR to PFR is represented by the region between the first-order and the second-order curves.

GENERAL GRAPHICAL COMPARISON

- For reactions with arbitrary but known rate, the performance capabilities of MFR and PFRs are best illustrated in Fig. 4-2.
- The ratio of shaded and of hatched areas gives the ratio of space-times needed in these two reactors.
- The rate curve in Fig. 4-2 is typical of the large class of reactions whose rate decreases continually on approach to equilibrium (for all nth-order reactions, n > 0).
- For such reactions it can be seen that MFR always needs a larger volume than does PFRs for any given duty.

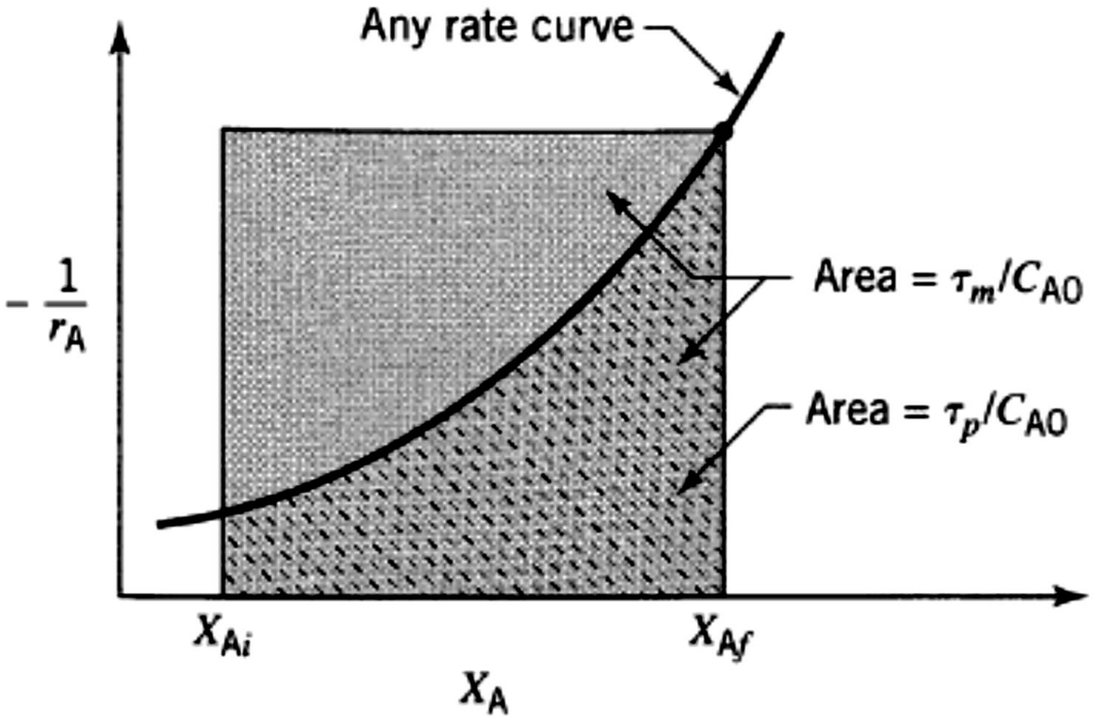


Figure 4-2 Comparison of performance of MFR and PFRs for any reaction kinetics.

MULTIPLE REACTOR SYSTEMS

- **Plug Flow Reactors in Series and/or in Parallel**
- Consider N plug flow reactors connected in series, and let X_1, X_2, . . . , X_N be the fractional conversion of component A leaving reactor 1, 2, . . . , N.
- Basing the material balance on the feed rate of A to the first reactor, we find for the i^th reactor that

$$\frac{V_i}{F_0} = \int_{X_{i-1}}^{X_i} \frac{dX}{-r} \qquad \text{4-5}$$

- Or for the N reactors in series

$$\frac{V}{F_0} = \sum_{i=1}^{N} \frac{V_i}{F_0} = \frac{V_1 + V_2 + \cdot \cdot \cdot + V_N}{F_0}$$

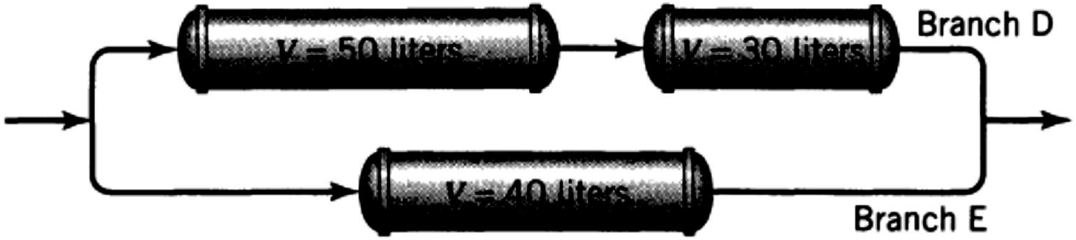
$$= \int_{X_0=0}^{X_1} \frac{dX}{-r} + \int_{X_1}^{X_2} \frac{dX}{-r} + \cdot \cdot \cdot + \int_{X_{N-1}}^{X_N} \frac{dX}{-r} = \int_0^{X_N} \frac{dX}{-r} \qquad \text{4-6}$$

- Hence, N plug flow reactors in series with a total volume V gives the same conversion as a single plug flow reactor of volume V.

GENERAL GRAPHICAL COMPARISON

- For the optimum hook up of PFRs connected in parallel or in any parallel-series combination, the whole system is treated as a single PFR of volume equal to the total volume of the individual units if the feed is distributed in such a manner that fluid streams that meet have the same composition.
- Thus, for reactors in parallel V/F or τ must be the same for each parallel line. Any other way of feeding is less efficient.

- EXAMPLE 1
- The reactor setup shown in the Figure below consists of three plug flow reactors in two parallel branches. Branch D has a reactor of volume 50 liters followed by a reactor of volume 30 liters. Branch E has a reactor of volume 40 liters. What fraction of the feed should go to branch D?



EXAMPLE 1 SOLUTION

- Branch D consists of two reactors in series; hence, it may be considered to be a single reactor of volume
- $$V_D = 50 + 30 = 80 \text{ liters}$$
- Now for reactors in parallel V/F must be identical if the conversion is to be the same in each branch. Therefore,

$$\left(\frac{V}{F}\right)_D = \left(\frac{V}{F}\right)_E$$

- or

$$\frac{F_D}{F_E} = \frac{V_D}{V_E} = \frac{80}{40} = \underline{\underline{2}}$$

- Therefore, two-thirds of the feed must be fed to branch D.

THANK YOU
FOR
YOUR
ATTENTION!
ANY QUESTIONS?