CHEN 416: CHEMICAL REACTION ENGINEERING II

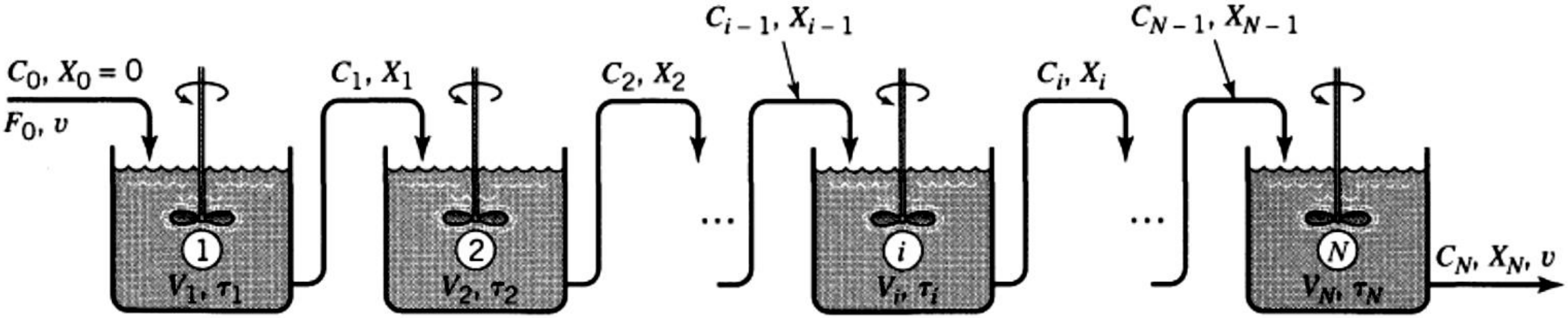
DESIGN OF MULTIPLE REACTORS FOR SINGLE REACTIONS

LEARNING OBJECTIVES

- At the end of this week's lecture, students should be able to:
  - Design and compare MFR and PFRs for single reactions
  - Design of multiple MFRs for single reactions
    - Equal-sized MFRs in series
    - Unequal sized MFRs in series

EQUAL-SIZE MIXED FLOW REACTORS IN SERIES

- In PFR, the concentration of reactant decreases progressively through the system, whereas in MFR, the concentration drops immediately to a low value.
- Hence, a PFR is more efficient than a MFR for reactions whose rates increase with reactant concentration, such as nth-order irreversible reactions, n > 0.
- Consider a system of N MFRs connected in series.



- Though the concentration is uniform in each reactor, there is a change in concentration as fluid moves from reactor to reactor.
- This stepwise drop in concentration suggests that the larger the number of units in series, the closer should the behavior of the system approach plug flow (as shown in Fig.4-3).

EQUAL-SIZE MIXED FLOW REACTORS IN SERIES

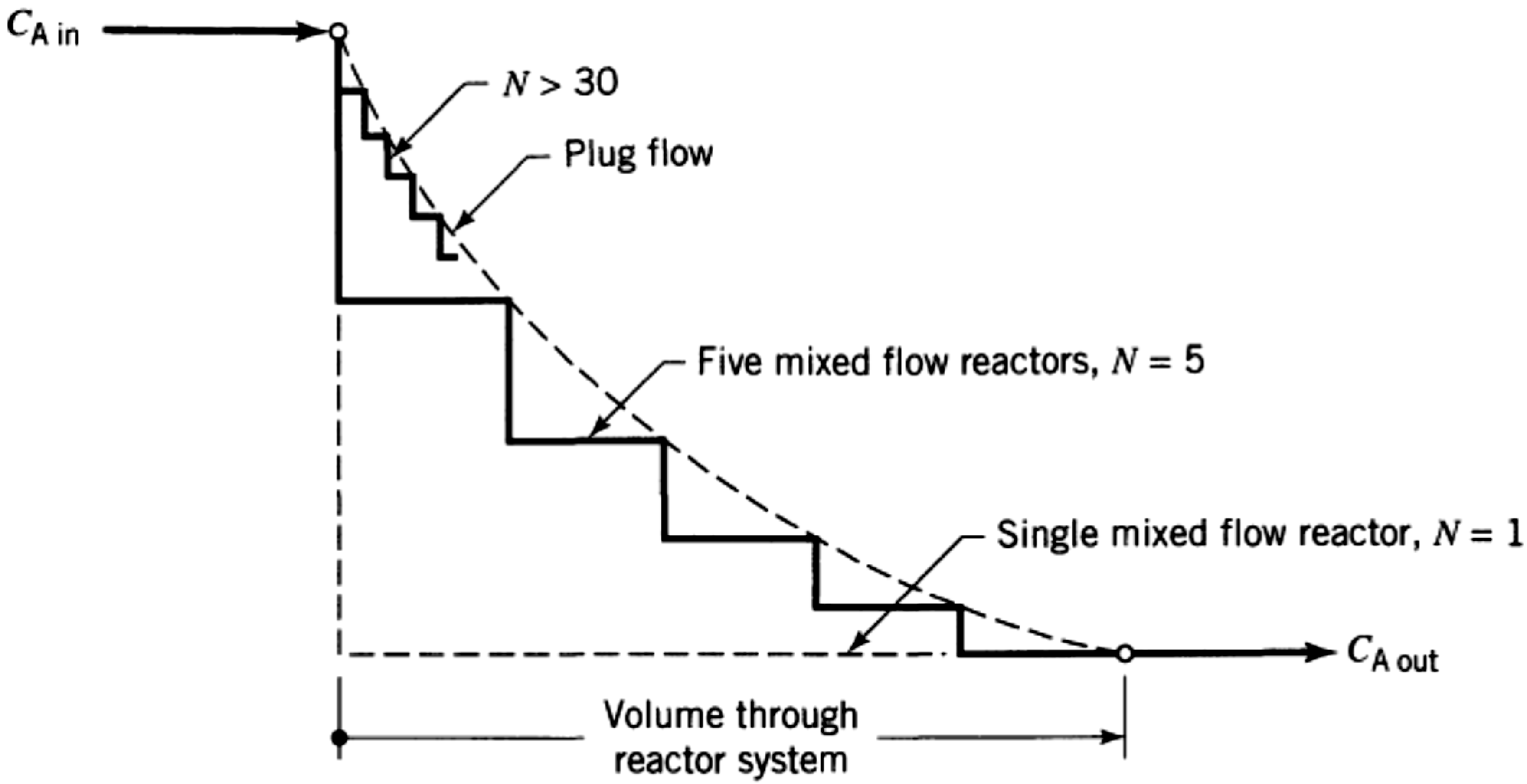


Figure 4-3 Concentration profile through an N-stage MFR system compared with single flow reactors.

EQUAL-SIZE MIXED FLOW REACTORS IN SERIES

- **For constant density first-order reactions.** From a material balance for component A about vessel i gives
- $$\tau_i = \frac{C_0 V_i}{F_0} = \frac{V_i}{v} = \frac{C_0(X_i - X_{i-1})}{-r_{Ai}} \qquad \text{4-7}$$
- Because Ɛ = 0 this may be written in terms of concentrations. Hence

$$\tau_i = \frac{C_0[(1 - C_i/C_0) - (1 - C_{i-1}/C_0)]}{kC_i} = \frac{C_{i-1} - C_i}{kC_i}$$

- Or $$\frac{C_{i-1}}{C_i} = 1 + k\tau_i \qquad \text{4-8}$$
- Now the space-time τ (or mean residence time *t*) is the same in all the equal size reactors of volume V_i. Therefore,
- $$\frac{C_0}{C_N} = \frac{1}{1 - X_N} = \frac{C_0}{C_1}\frac{C_1}{C_2}\cdots\frac{C_{N-1}}{C_N} = (1 + k\tau_i)^N \qquad \text{4-9a}$$
- Rearranging, we find for the system as a whole
- $$\tau_{N\,\text{reactors}} = N\tau_i = \frac{N}{k}\left[\left(\frac{C_0}{C_N}\right)^{1/N} - 1\right] \qquad \text{4-9b}$$

EQUAL-SIZE MIXED FLOW REACTORS IN SERIES

- In the limit, for N ⟶ ∞, this equation reduces to the PFR equation

- $$\tau_p = \frac{1}{k} \ln \frac{C_0}{C} \qquad 4\text{-}10$$

- With Eqs.4-9b and 4-10 we can compare performance of N reactors in series with a PFR or with a single MFR.

- This comparison is shown in Fig. 4-4 for first-order reactions in which density variations are negligible.

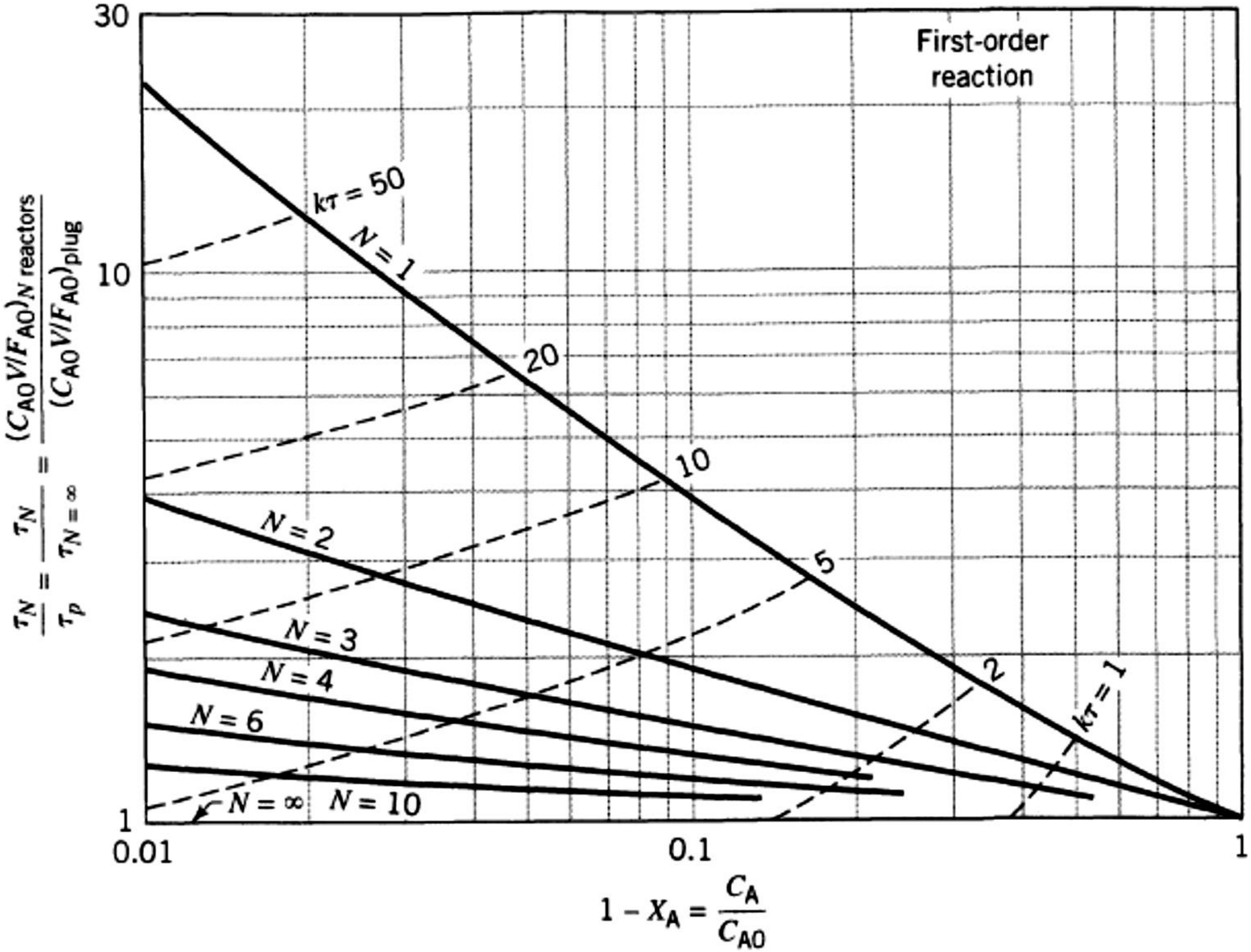
- **Second-Order Reactions.**

- The performance of a series of MFRs for a second-order, bimolecular-type reaction, no excess of either reactant, may be evaluated by a procedure similar to that of a first-order reaction.

- Thus, for N reactors in series we find

- $$C_N = \frac{1}{4k\tau_i}\left(-2 + 2\underbrace{\sqrt{-1 \cdots + 2\sqrt{-1 + 2\sqrt{1 + 4C_0 k\tau_i}}}}_{\vdots\ \} N}\right) \qquad 4\text{-}11$$

- whereas for plug flow



N.B: For the same processing rate of identical feed the ordinate measures the volume ratio V_N/V_P directly

Fig.4-4: Comparison of performance of a series of N equal-sized MFRs with a PFR for the 1st order reactions

$$\frac{C_0}{C} = 1 + C_0 k \tau_p$$

- A comparison of the performance of these reactors is shown in Fig. 4-5.
- For the same processing rate of identical feed the ordinate measures the volume ratio V_N/V_P directly or space-time ratio V_N/V_P directly.

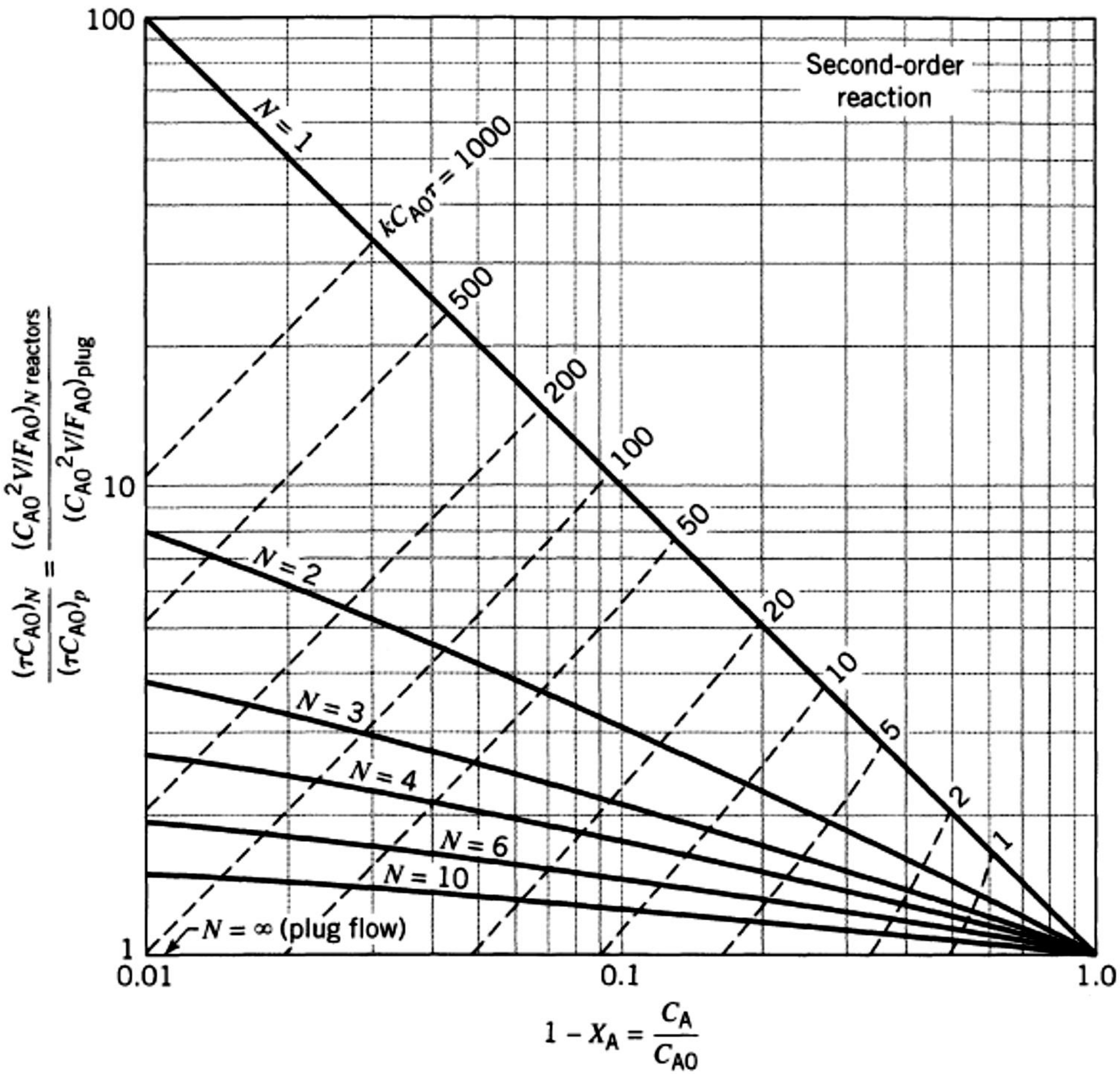


Fig.4-5: Comparison of performance of a series of N equal-sized MFRs with a PFR for the 2nd order reactions with negligible expansion

EXAMPLE L5-1

At present 90% of reactant A is converted into product by a second-order reaction in a single mixed flow reactor. A second reactor similar to the one being used is planned to be placed in series with it.

a) For the same treatment rate as that used at present, how will this addition affect the conversion of reactant?

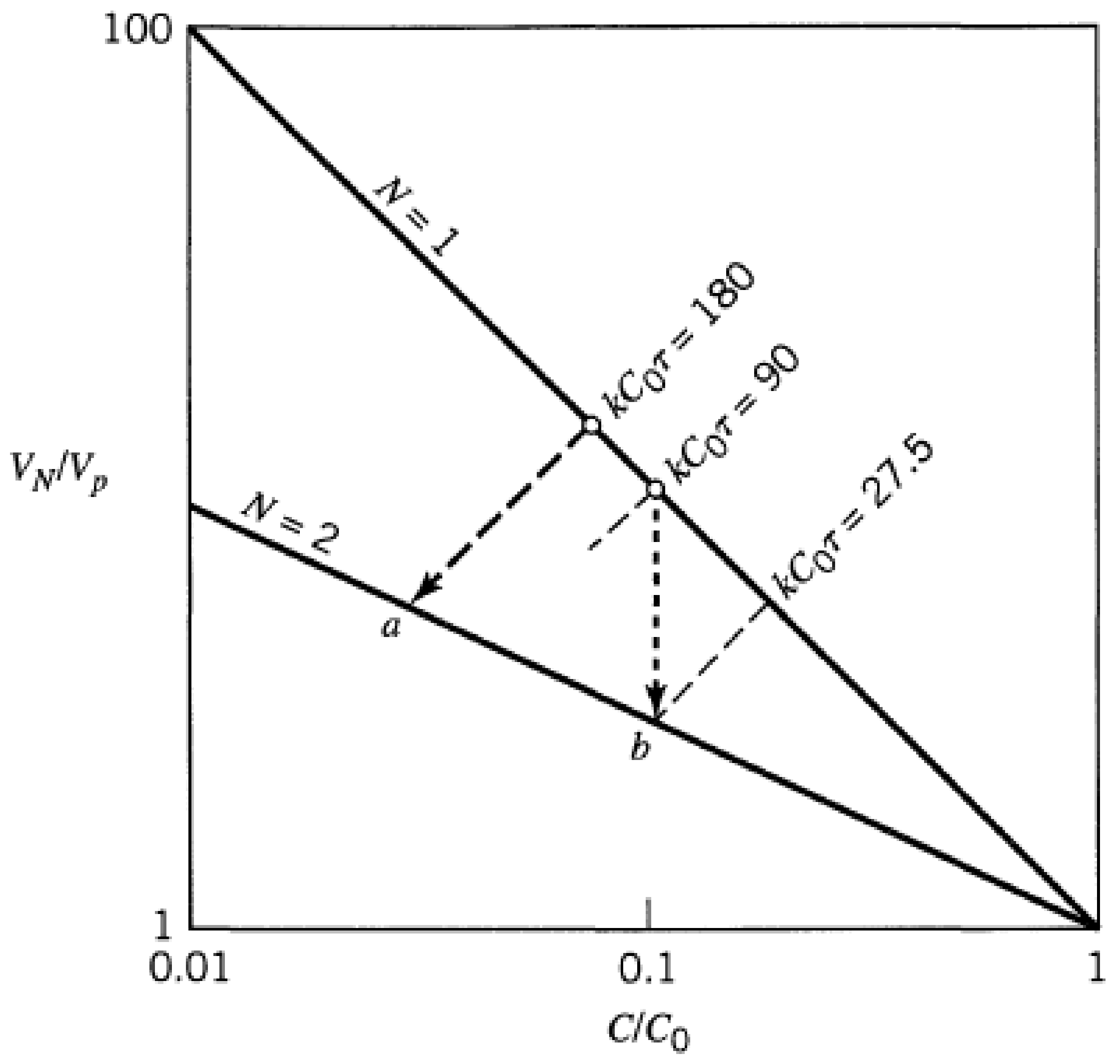
b) For the same 90% conversion, by how much can the treatment rate be increased?

- SOLUTION

(a) Find the conversion for the same treatment rate. For the single reactor at 90% conversion we have from Fig. 4-5b

- $$kC_0\tau = 90$$
- For the two reactors the space-time or holding time is doubled; hence, the operation will be represented by the dashed line of Fig. 4-5b where
- $$kC_0\tau = 180$$
- This line cuts the N = 2 line at a conversion X = 97.4%, point a.

EXAMPLE 1 SOLUTION



EXAMPLE L5-1 SOLUTION

(b) Find the treatment rate for the same conversion. Staying on the 90% conversion line, we find for N = 2 that

- $kC_0\tau = 27.5$, point b
- Comparing the value of the reaction rate group for N = 1 and N = 2, we find

$$\frac{(kC_0\tau)_{N=2}}{(kC_0\tau)_{N=1}} = \frac{\tau_{N=2}}{\tau_{N=1}} = \frac{(V/v)_{N=2}}{(V/v)_{N=1}} = \frac{27.5}{90}$$

- Since V,=, = 2V,,, the ratio of flow rates becomes

$$\frac{v_{N=1}}{v_{N=1}} = \frac{90}{27.5}(2) = 6.6$$

- Thus, the treatment rate can be raised to 6.6 times the original.
- ***Note.*** If the second reactor had been operated in parallel with the original unit then the treatment rate could only be doubled. Thus, there is a definite advantage in operating these two units in series. This advantage becomes more pronounced at higher conversions.

MIXED FLOW REACTORS OF DIFFERENT SIZES IN SERIES

- For kinetics in MFRs of different size, two questions may be asked:
  - how to find the outlet conversion from a given reactor system,
  - how to find the best setup to achieve a given conversion.
- Different procedures are used for these two problems.

- **Finding the Conversion in a Given System**
- R.W. Jones (1951) presented a graphical procedure for determining the outlet composition from a series of MFRs of various sizes for reactions with negligible density change.
  - All that is needed is an ***r*** **vs C** curve for component A to represent the reaction rate at various concentrations.
- Let's consider 3 MFRs in series with volumes, feed rates, concentrations, space-times (equal to residence times because $\varepsilon_A = 0$), and volumetric flow rates as shown in Fig. 4-6.

MIXED FLOW REACTORS OF DIFFERENT SIZES IN SERIES

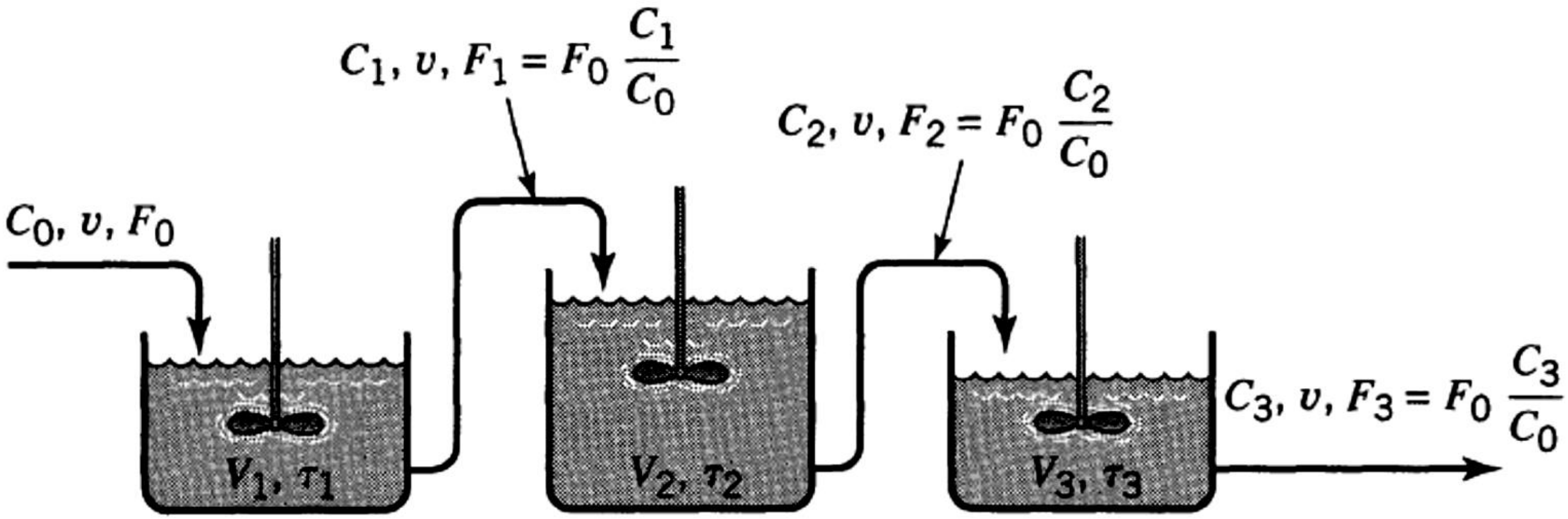


Figure 4-6 Notation for a series of unequal-size mixed flow reactors

- Now from the performance equation for MFR, noting that $\varepsilon_A = 0$, we may write for component **A** in the first reactor that

- $$\tau_1 = \bar{t}_1 = \frac{V_1}{v} = \frac{C_0 - C_1}{(-r)_1} \qquad \text{or} \qquad -\frac{1}{\tau_1} = \frac{(-r)_1}{C_1 - C_0}$$

- Similarly for the ith reactor

$$-\frac{1}{\tau_i} = \frac{(-r)_i}{C_i - C_{i-1}}$$

MIXED FLOW REACTORS OF DIFFERENT SIZES IN SERIES

- A plot of C vs r yields the curve of Fig.4-7 for component A.
- To find the conditions in the first reactor,
  - the inlet concentration C_0 is known (point L),
  - C_1 and $(-r)_1$ correspond to a point on the curve to be found (point M),
  - and that the slope of the line LM = MN/NL
  - from C_0 draw a line of slope $-(1/\tau_1)$ until it cuts the rate curve; this gives C_1.
  - Similarly, a line of slope $-(1/\tau_2)$ from point N cuts the curve at P, giving C_2 of material leaving the second reactor.
  - This procedure is then repeated as many times as needed.

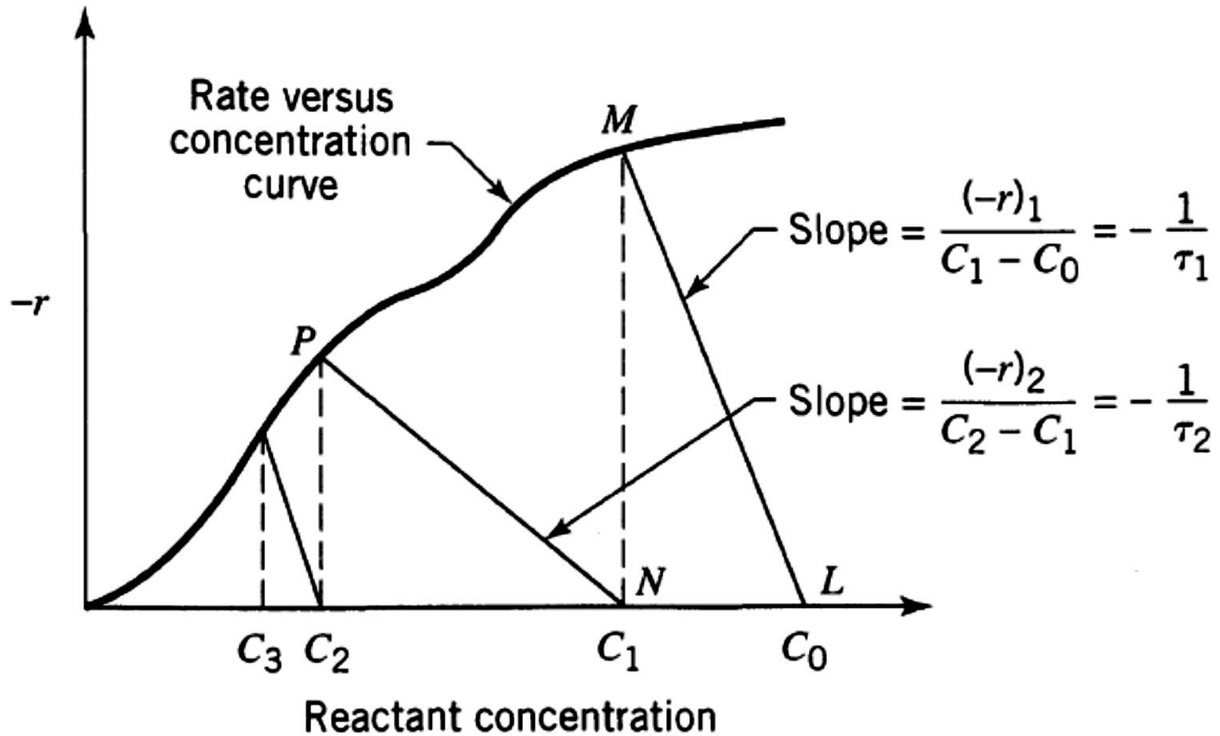


Figure 4-7 Graphical procedure for finding compositions in a series of mixed flow reactors.

- With slight modification this graphical method can be extended to reactions in which density changes are appreciable.

MIXED FLOW REACTORS OF DIFFERENT SIZES IN SERIES

- **Determining the Best System for a Given Conversion.**
- Suppose we want to find the minimum size of two MFRs in series to achieve a specified conversion of feed which reacts with arbitrary but known kinetics.
- The basic performance expressions gives for the first and second reactors.
- $$\frac{\tau_1}{C_0} = \frac{X_1}{(-r)_1} \quad \text{and} \quad \frac{\tau_2}{C_0} = \frac{X_2 - X_1}{(-r)_2}$$
- These relationships are displayed in Fig. 4-8 for two alternative reactor arrangements, both giving the same final conversion X_2. Note, as the intermediate conversion X_1 changes, so does the size ratio of the units (represented by the two shaded areas) as well as the total volume of the two vessels required (the total area shaded).
- Figure 4-8 shows that the total reactor volume is as small as possible (total shaded area is minimized) when the rectangle KLMN is as large as possible.
- To maximize the area of rectangle KLMN, X_1 position (or point M on the curve) would have to be chosen.

MIXED FLOW REACTORS OF DIFFERENT SIZES IN SERIES

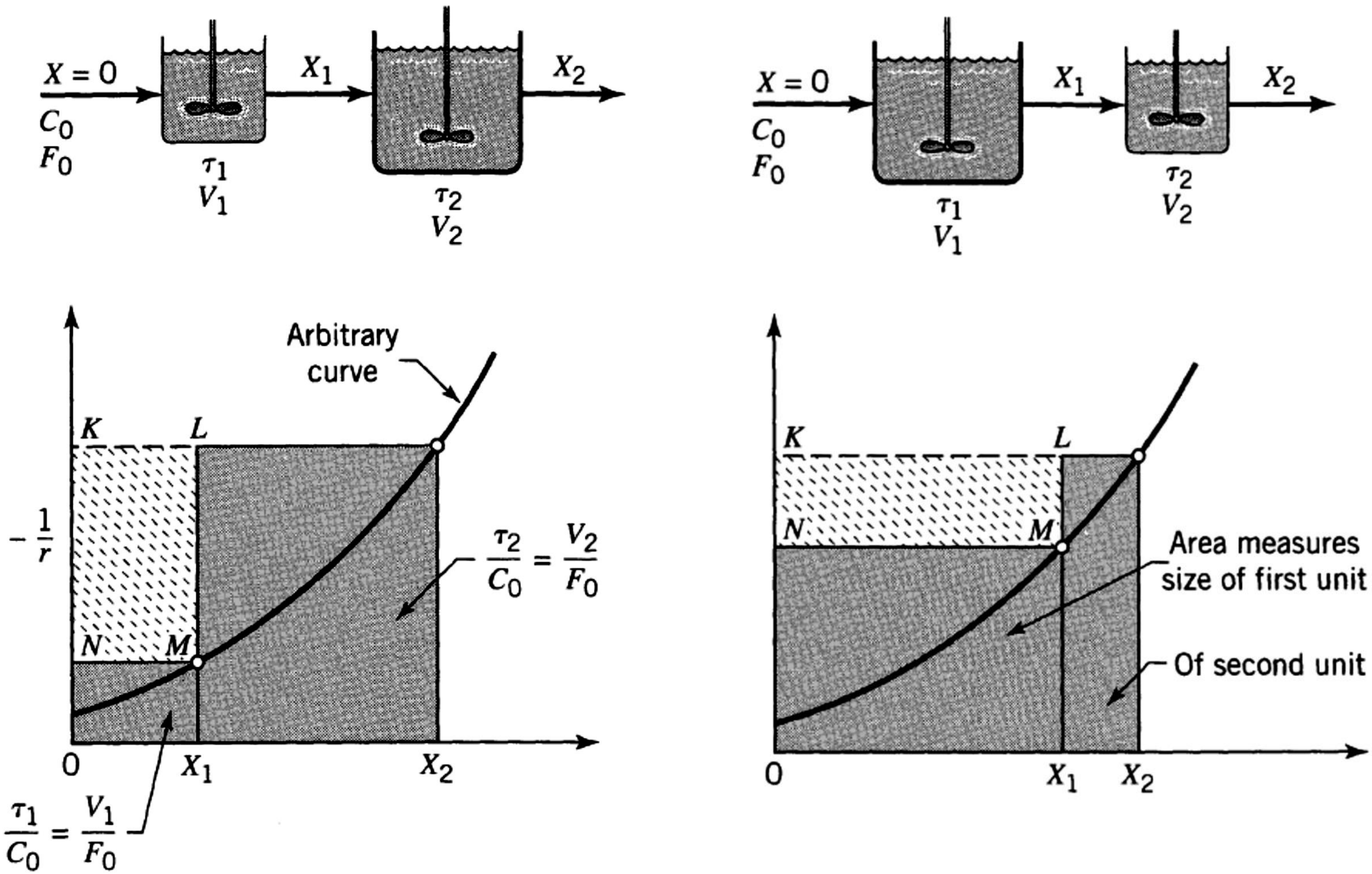


Figure 4-8 Graphical representation of the variables for two mixed flow reactors in series.

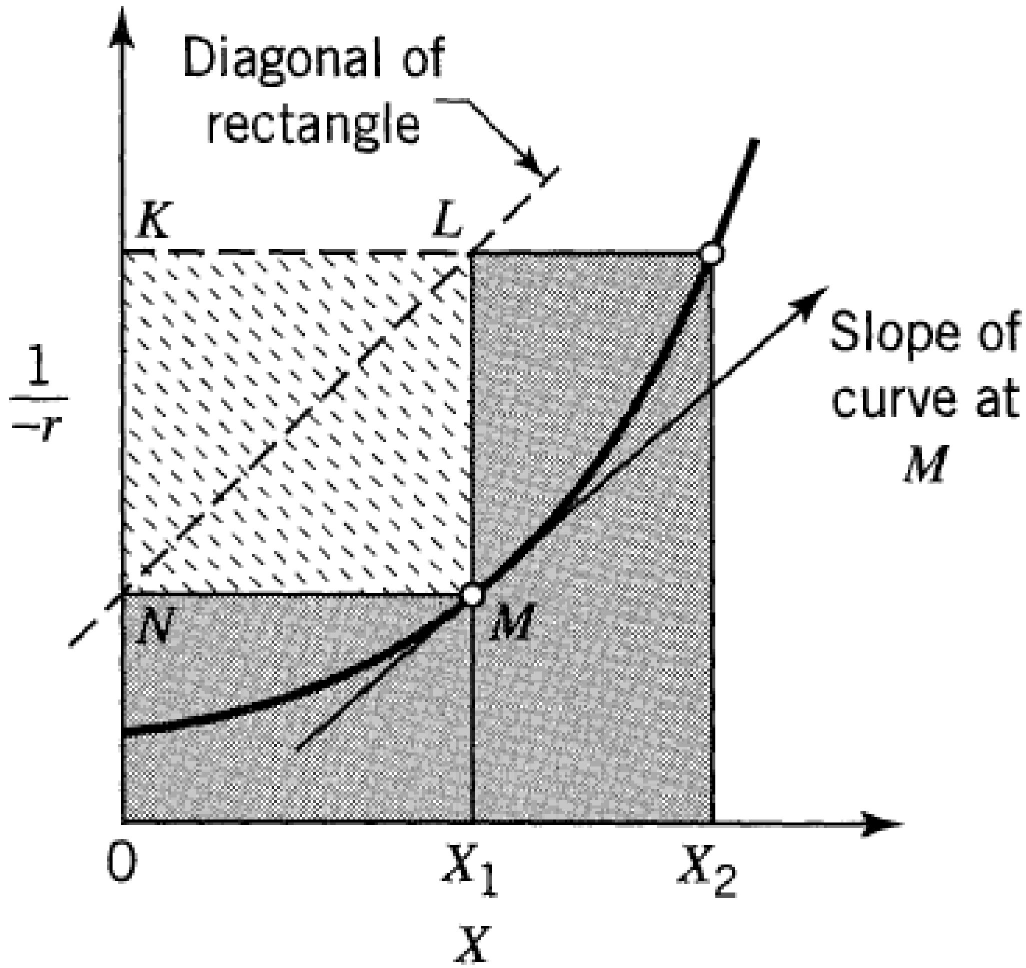


Figure 4-9 Maximization of rectangles applied to find the optimum intermediate conversion and optimum sizes of two mixed flow reactors in series.

MIXED FLOW REACTORS OF DIFFERENT SIZES IN SERIES

- The optimum size ratio for the two MFRs in series is found in general to be dependent on the kinetics of the reaction and on the conversion level.
- For the case of first-order reactions, equal-size reactors are best;
  - for $n > 1$, the smaller reactor should come first; and
  - for $n < 1$, the larger should come first.
- However, the advantage of the minimum size system over the equal-size system is quite small, only a few percent at most.
- Hence, overall economic consideration would nearly always recommend using equal-size units.
- The above procedure can be extended directly to multistage operations; however, the argument for equal-size units is stronger still than for the two-stage system.

REACTORS OF DIFFERENT TYPES IN SERIES

- If reactors of different types are put in series, such as a MFR followed by a PFR which in turn is followed by another MFR, we may write for the three reactors

$$\frac{V_1}{F_0} = \frac{X_1 - X_0}{(-r)_1}, \quad \frac{V_2}{F_0} = \int_{X_1}^{X_2} \frac{dX}{-r}, \quad \frac{V_3}{F_0} = \frac{X_3 - X_2}{(-r)_3}$$

- These relationships are represented in graphical form in Fig. 4-10

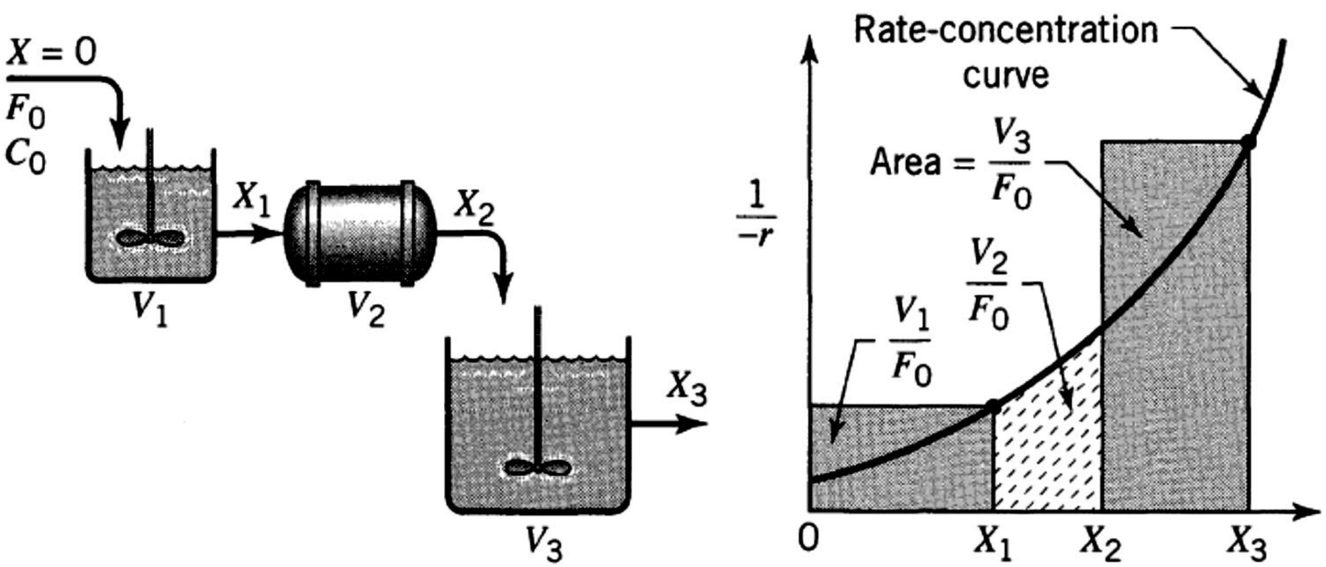


Figure 4-10 Graphical design procedure for reactors in series.

This allows the prediction of the overall conversions for such systems, or conversions at intermediate points between the individual reactors, which may be needed to determine the duty of inter-stage heat exchangers.

REACTORS OF DIFFERENT TYPES IN SERIES

- **General Rules for the Best Arrangement of a Set of Ideal Reactors.**

1. For a reaction any nth-order reaction, n > 0 (whose rate-concentration curve rises monotonically),
   - the reactors should be connected in series.
   - They should be ordered so as to keep the concentration of reactant as high as possible if the rate-concentration curve is concave (n > I),
   - and as low as possible if the curve is convex (n < 1).
   - As an example, for the case of Fig. 4-10 the ordering of units should be plug, small mixed, large mixed, for n > 1; the reverse order should be used when *n* < 1.

2. For reactions where the rate-concentration curve passes through a maximum or minimum the arrangement of units depends on the actual shape of curve, the conversion level desired, and the units available. No simple rules can be suggested.

3. Whatever may be the kinetics and the reactor system, an examination of the $1/(-r_A)$ vs C_A curve is a good way to find the best arrangement of units.

THANK YOU
FOR
YOUR
ATTENTION!
ANY QUESTIONS?