

Figure 6.2 Comparison of performance of mixed flow and plug flow reactors for any reaction kinetics.

General Graphical Comparison

For reactions with arbitrary but known rate the performance capabilities of mixed and plug flow reactors are best illustrated in Fig. 6.2. The ratio of shaded and of hatched areas gives the ratio of space-times needed in these two reactors.

The rate curve drawn in Fig. 6.2 is typical of the large class of reactions whose rate decreases continually on approach to equilibrium (this includes all n th-order reactions, $n > 0$). For such reactions it can be seen that mixed flow always needs a larger volume than does plug flow for any given duty.

6.2 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, \dots, X_N be the fractional conversion of component A leaving reactor 1, 2, \dots , N . Basing the material balance on the feed rate of A to the first reactor, we find for the i th reactor from Eq. 5.18

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

or for the N reactors in series

$$\begin{aligned} \frac{V}{F_0} &= \sum_{i=1}^N \frac{V_i}{F_0} = \frac{V_1 + V_2 + \dots + V_N}{F_0} \\ &= \int_{X_0=0}^{X_1} \frac{dX}{-r} + \int_{X_1}^{X_2} \frac{dX}{-r} + \dots + \int_{X_{N-1}}^{X_N} \frac{dX}{-r} = \int_0^{X_N} \frac{dX}{-r} \end{aligned}$$

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 .

For the optimum hook up of plug flow reactors connected in parallel or in any parallel-series combination, we can treat the whole system as a single plug flow reactor 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 6.1 OPERATING A NUMBER OF PLUG FLOW REACTORS

The reactor setup shown in Fig. E6.1 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?

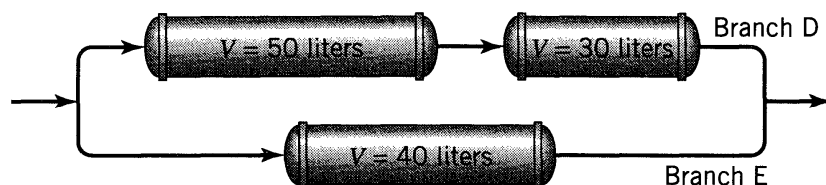


Figure E6.1

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

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

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

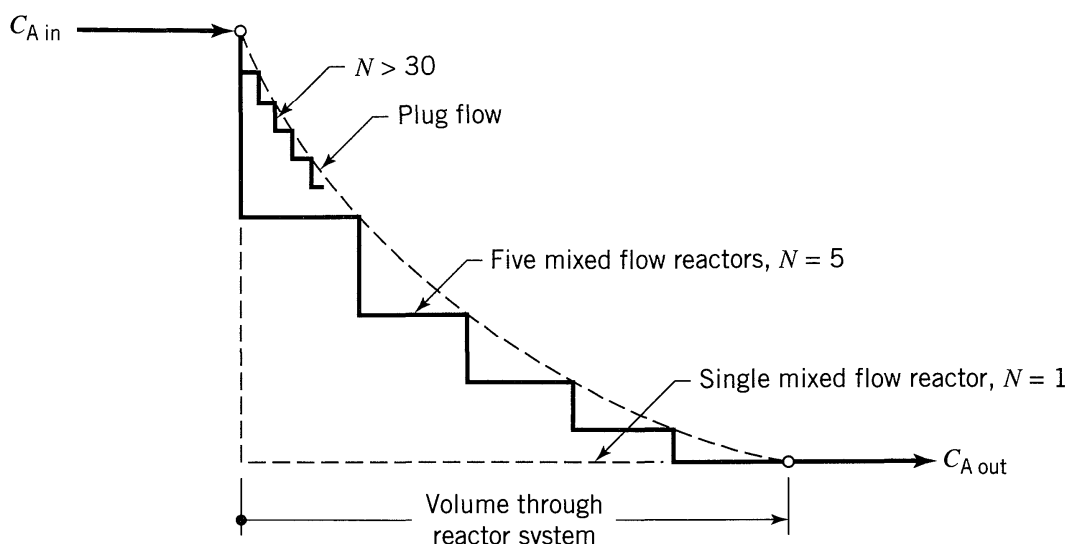


Figure 6.3 Concentration profile through an N -stage mixed flow reactor system compared with single flow reactors.

Equal-Size Mixed Flow Reactors in Series

In plug flow, the concentration of reactant decreases progressively through the system; in mixed flow, the concentration drops immediately to a low value. Because of this fact, a plug flow reactor is more efficient than a mixed flow reactor for reactions whose rates increase with reactant concentration, such as n th-order irreversible reactions, $n > 0$.

Consider a system of N mixed flow reactors connected in series. Though the concentration is uniform in each reactor, there is, nevertheless, a change in concentration as fluid moves from reactor to reactor. This stepwise drop in concentration, illustrated in Fig. 6.3, suggests that the larger the number of units in series, the closer should the behavior of the system approach plug flow. This will be shown to be so.

Let us now quantitatively evaluate the behavior of a series of N equal-size mixed flow reactors. Density changes will be assumed to be negligible; hence $\varepsilon = 0$ and $t = \tau$. As a rule, with mixed flow reactors it is more convenient to develop the necessary equations in terms of concentrations rather than fractional conversions; therefore, we use this approach. The nomenclature used is shown in Fig. 6.4 with subscript i referring to the i th vessel.

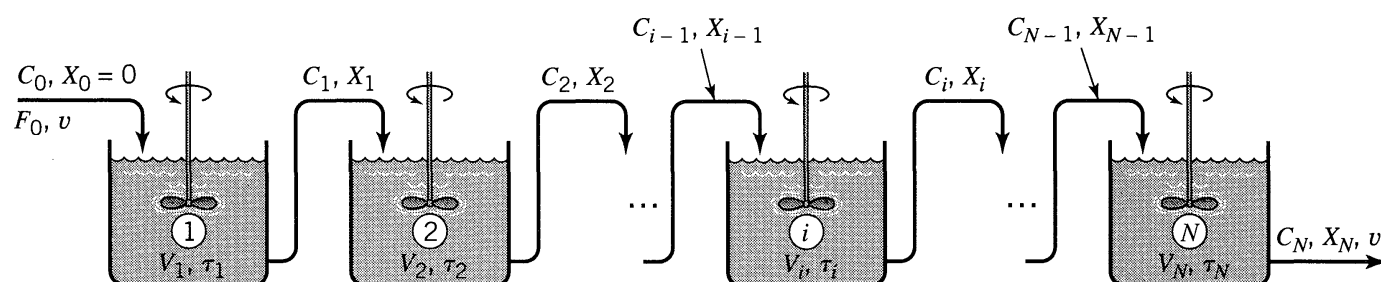


Figure 6.4 Notation for a system of N equal-size mixed reactors in series.

First-Order Reactions. From Eq. 5.12 a material balance for component A about vessel i gives

$$\tau_i = \frac{C_0 V_i}{F_0} = \frac{V_i}{v} = \frac{C_0(X_i - X_{i-1})}{-r_{Ai}}$$

Because $\varepsilon = 0$ 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

$$\frac{C_{i-1}}{C_i} = 1 + k\tau_i \quad (5)$$

Now the space-time τ (or mean residence time t) is the same in all the equal-size reactors of volume V_i . Therefore,

$$\frac{C_0}{C_N} = \frac{1}{1 - X_N} = \frac{C_0 C_1}{C_1 C_2} \cdots \frac{C_{N-1}}{C_N} = (1 + k\tau_i)^N \quad (6a)$$

Rearranging, we find for the system as a whole

$$\tau_{N \text{ reactors}} = N\tau_i = \frac{N}{k} \left[\left(\frac{C_0}{C_N} \right)^{1/N} - 1 \right] \quad (6b)$$

In the limit, for $N \rightarrow \infty$, this equation reduces to the plug flow equation

$$\tau_p = \frac{1}{k} \ln \frac{C_0}{C} \quad (7)$$

With Eqs. 6b and 7 we can compare performance of N reactors in series with a plug flow reactor or with a single mixed flow reactor. This comparison is shown in Fig. 6.5 for first-order reactions in which density variations are negligible.

Second-Order Reactions. We may evaluate the performance of a series of mixed flow reactors for a second-order, bimolecular-type reaction, no excess of either reactant, by a procedure similar to that of a first-order reaction. Thus, for

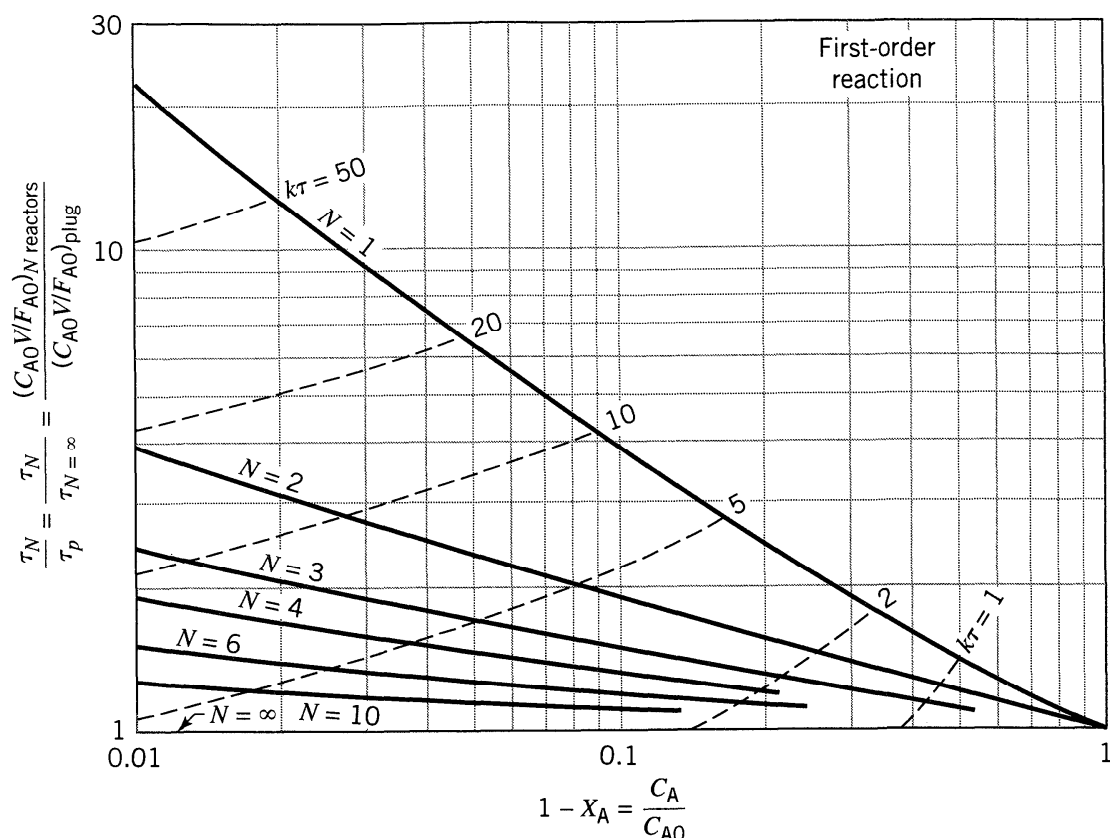


Figure 6.5 Comparison of performance of a series of N equal-size mixed flow reactors with a plug flow reactor for the first-order reaction



For the same processing rate of identical feed the ordinate measures the volume ratio V_N/V_p directly.

N reactors in series we find

$$C_N = \frac{1}{4k\tau_i} \left(-2 + 2 \sqrt{-1 \cdots + 2 \sqrt{-1 + 2 \sqrt{1 + 4C_0 k\tau_i}}} \right) N \quad (8a)$$

whereas for plug flow

$$\frac{C_0}{C} = 1 + C_0 k\tau_p \quad (8b)$$

A comparison of the performance of these reactors is shown in Fig. 6.6.

Figures 6.5 and 6.6 support our intuition by showing that the volume of system required for a given conversion decreases to plug flow volume as the number of reactors in series is increased, the greatest change taking place with the addition of a second vessel to a one-vessel system.

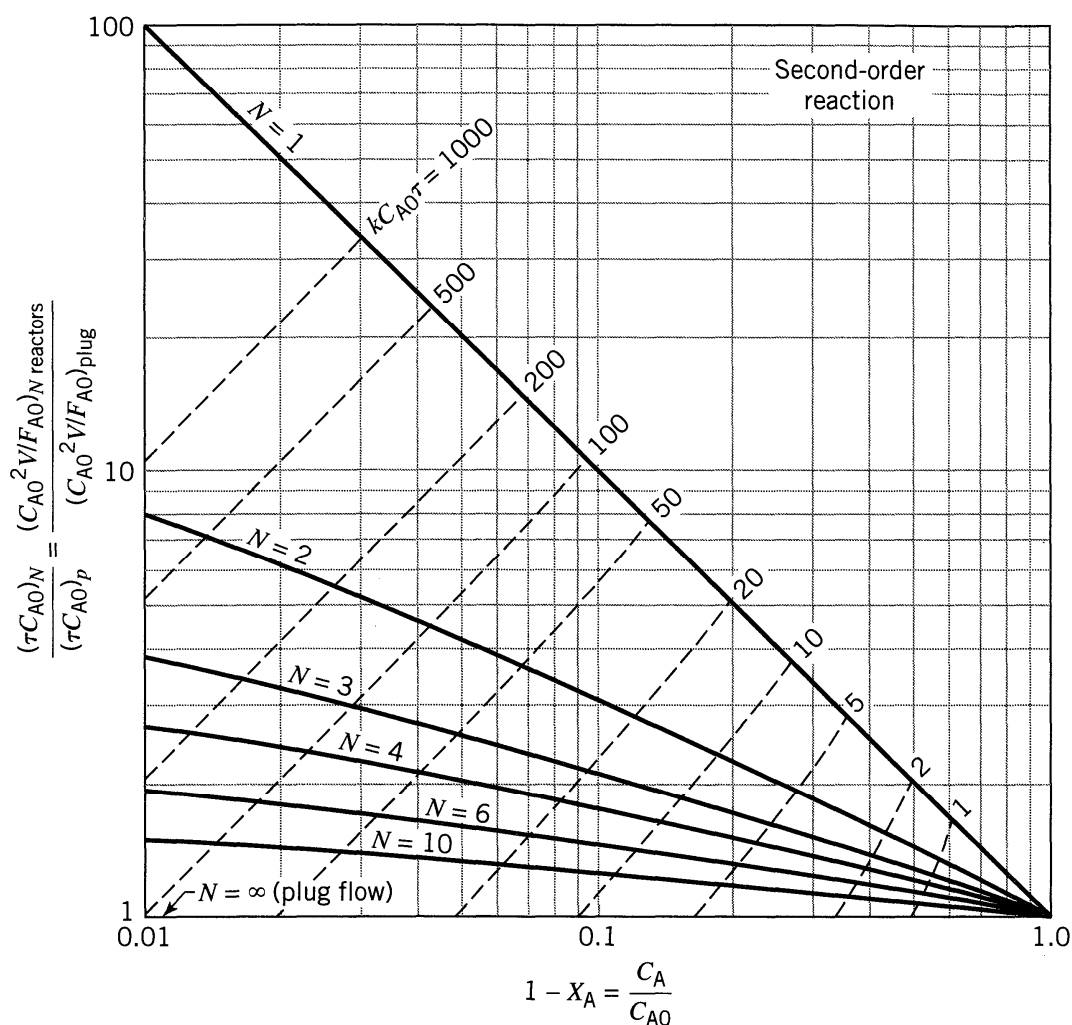
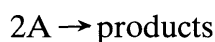


Figure 6.6 Comparison of performance of a series of N equal-size mixed flow reactors with a plug flow reactor for elementary second-order reactions



with negligible expansion. For the same processing rate of identical feed the ordinate measures the volume ratio V_N/V_p or space-time ratio τ_N/τ_p directly.

EXAMPLE 6.2 MIXED FLOW REACTORS IN SERIES

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

- For the same treatment rate as that used at present, how will this addition affect the conversion of reactant?
- For the same 90% conversion, by how much can the treatment rate be increased?

SOLUTION

The sketch of Fig. E6.2 shows how the performance chart of Fig. 6.6 can be used to help solve this problem.

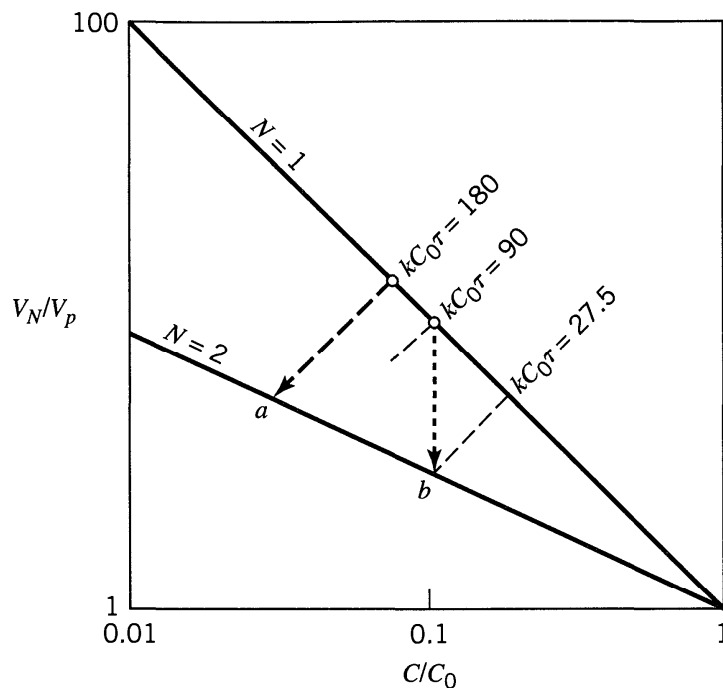


Figure E6.2

(a) Find the conversion for the same treatment rate. For the single reactor at 90% conversion we have from Fig. 6.6

$$kC_0\tau = 90$$

For the two reactors the space-time or holding time is doubled; hence, the operation will be represented by the dashed line of Fig. 6.6 where

$$kC_0\tau = 180$$

This line cuts the $N = 2$ line at a conversion $X = 97.4\%$, point *a*.

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

$$kC_0\tau = 27.5, \quad \text{point } b$$

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 $V_{N=2} = 2V_{N=1}$ 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 arbitrary kinetics in mixed flow reactors of different size, two types of questions may be asked: how to find the outlet conversion from a given reactor system, and the inverse question, how to find the best setup to achieve a given conversion. Different procedures are used for these two problems. We treat them in turn.

Finding the Conversion in a Given System A graphical procedure for finding the outlet composition from a series of mixed flow reactors of various sizes for reactions with negligible density change has been presented by Jones (1951). All that is needed is an r versus C curve for component A to represent the reaction rate at various concentrations.

Let us illustrate the use of this method by considering three mixed flow reactors in series with volumes, feed rates, concentrations, space-times (equal to residence times because $\varepsilon = 0$), and volumetric flow rates as shown in Fig. 6.7. Now from Eq. 5.11, noting that $\varepsilon = 0$, we may write for component A in the first reactor

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

or

$$-\frac{1}{\tau_1} = \frac{(-r)_1}{C_1 - C_0} \quad (9)$$

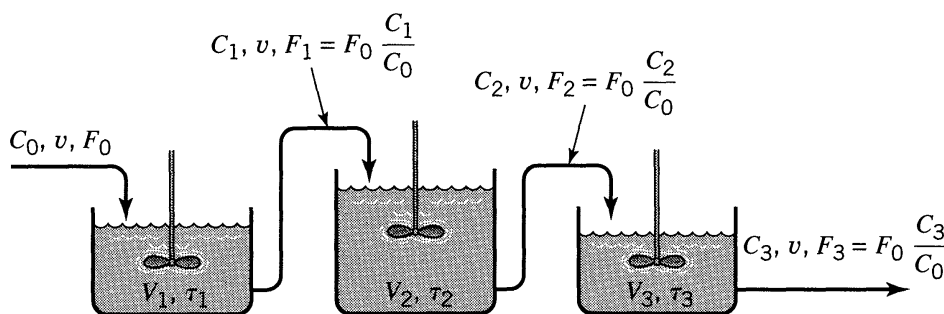


Figure 6.7 Notation for a series of unequal-size mixed flow reactors.

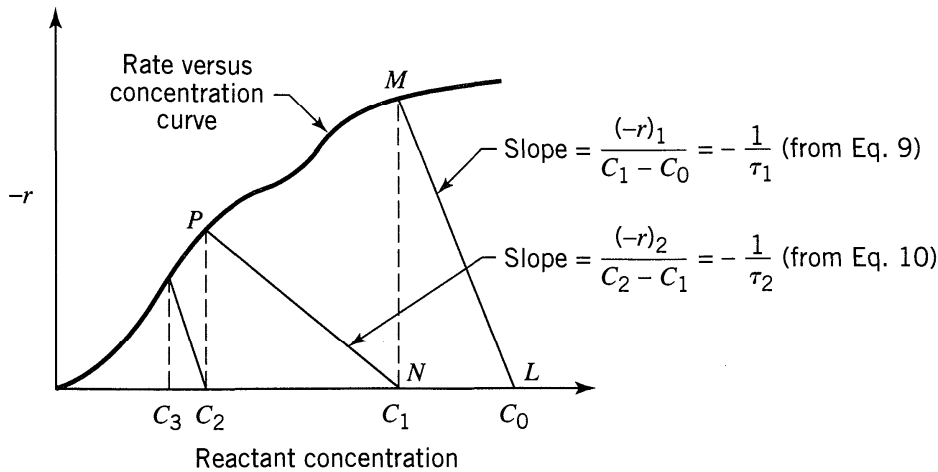


Figure 6.8 Graphical procedure for finding compositions in a series of mixed flow reactors.

Similarly, from Eq. 5.12 for the i th reactor we may write

$$-\frac{1}{\tau_i} = \frac{(-r)_i}{C_i - C_{i-1}} \quad (10)$$

Plot the C versus r curve for component A and suppose that it is as shown in Fig. 6.8. To find the conditions in the first reactor note that the inlet concentration C_0 is known (point L), that C_1 and $(-r)_1$ correspond to a point on the curve to be found (point M), and that the slope of the line $LM = MN/NL = (-r)_1 / (C_1 - C_0) = -(1/\tau_1)$ from Eq. 6.9. Hence, from C_0 draw a line of slope $-(1/\tau_1)$ until it cuts the rate curve; this gives C_1 . Similarly, we find from Eq. 6.10 that a line of slope $-(1/\tau_2)$ from point N cuts the curve at P , giving the concentration C_2 of material leaving the second reactor. This procedure is then repeated as many times as needed.

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

Determining the Best System for a Given Conversion. Suppose we want to find the minimum size of two mixed flow reactors in series to achieve a specified conversion of feed which reacts with arbitrary but known kinetics. The basic performance expressions, Eqs. 5.11 and 5.12, then give, in turn, for the first reactor

$$\frac{\tau_1}{C_0} = \frac{X_1}{(-r)_1} \quad (11)$$

and for the second reactor

$$\frac{\tau_2}{C_0} = \frac{X_2 - X_1}{(-r)_2} \quad (12)$$

These relationships are displayed in Fig. 6.9 for two alternative reactor arrangements, both giving the same final conversion X_2 . Note, as the intermediate

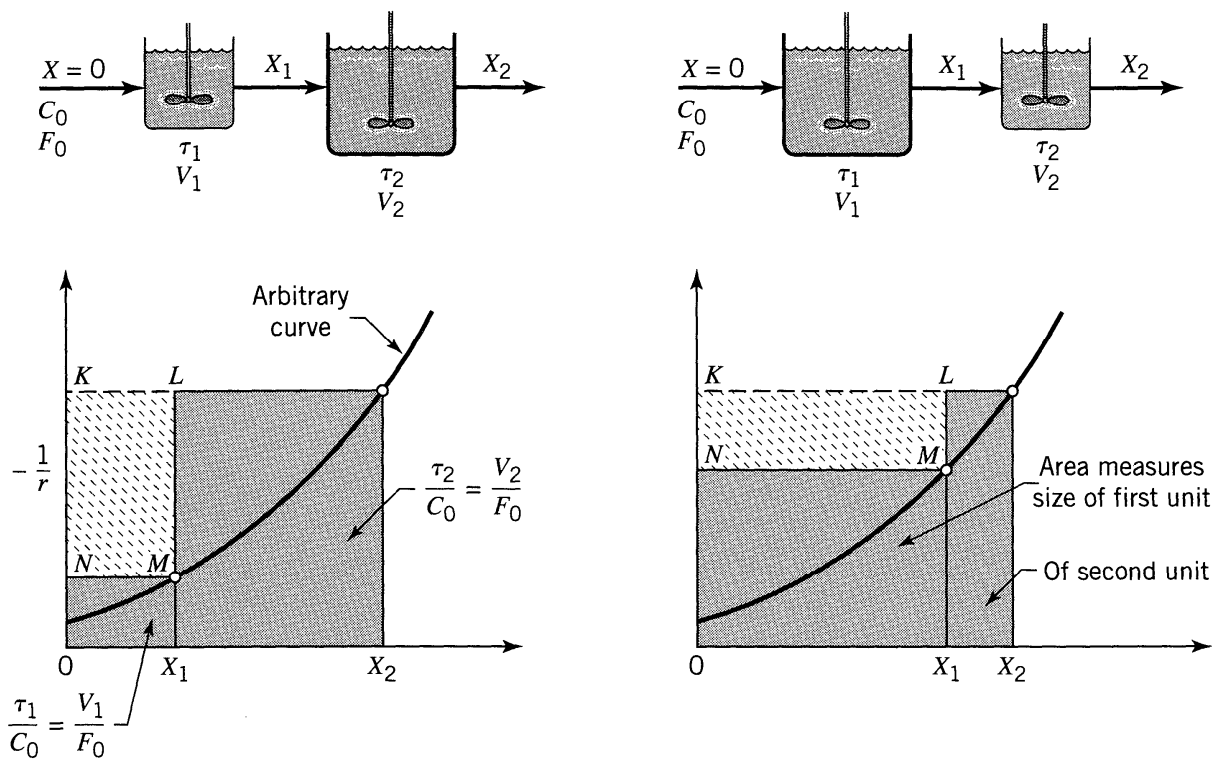


Figure 6.9 Graphical representation of the variables for two mixed flow reactors in series.

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 6.9 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. This brings us to the problem of choosing X_1 (or point M on the curve) so as to maximize the area of this rectangle. Consider this general problem.

Maximization of Rectangles. In Fig. 6.10, construct a rectangle between the x - y axes and touching the arbitrary curve at point $M(x, y)$. The area of the rectangle is then

$$A = xy \quad (13)$$

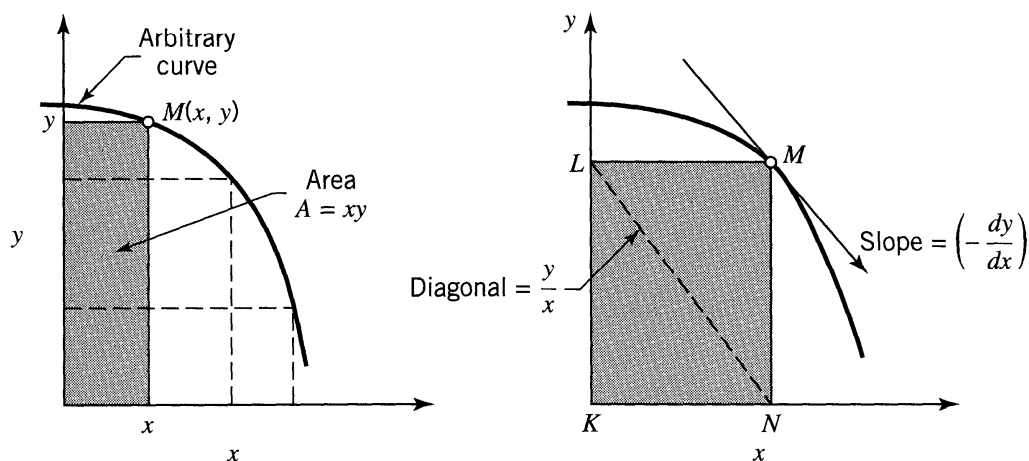


Figure 6.10 Graphical procedure for maximizing the area of a rectangle.

This area is maximized when

$$dA = 0 = y \, dx + x \, dy$$

or when

$$-\frac{dy}{dx} = \frac{y}{x} \quad (14)$$

In words, this condition means that the area is maximized when M is at that point where the slope of the curve equals the slope of the diagonal NL of the rectangle. Depending on the shape of the curve, there may be more than one or there may be no “best” point. However, for n th-order kinetics, $n > 0$, there always is just one “best” point.

We will use this method of maximizing a rectangle in later chapters. But let us return to our problem.

The optimum size ratio of the two reactors is achieved where the slope of the rate curve at M equals the diagonal NL . The best value of M is shown in Fig. 6.11, and this determines the intermediate conversion X_1 as well as the size of units needed.

The optimum size ratio for two mixed flow reactors in series is found in general to be dependent on the kinetics of the reaction and on the conversion level. For the special case of first-order reactions equal-size reactors are best; for reaction orders $n > 1$ the smaller reactor should come first; for $n < 1$ the larger should come first (see Problem 6.3). However, Szepe and Levenspiel (1964) show that 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, here the argument for equal-size units is stronger still than for the two-stage system.

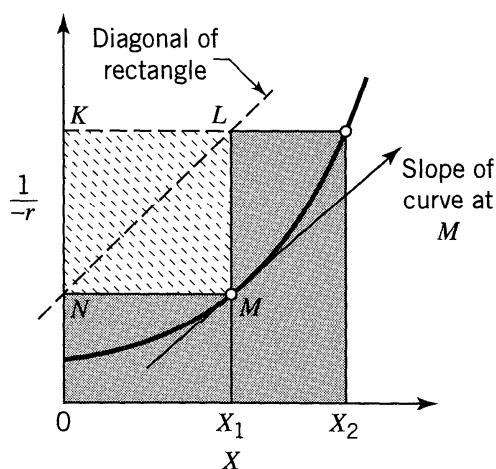


Figure 6.11 Maximization of rectangles applied to find the optimum intermediate conversion and optimum sizes of two mixed flow reactors in series.

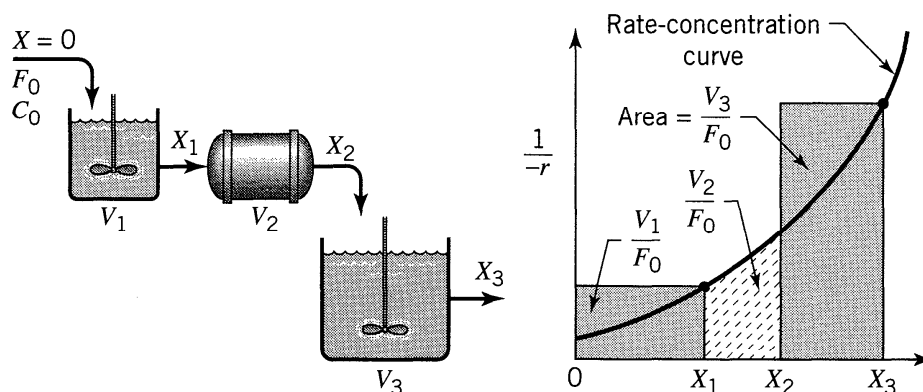


Figure 6.12 Graphical design procedure for reactors in series.

Reactors of Different Types in Series

If reactors of different types are put in series, such as a mixed flow reactor followed by a plug flow reactor which in turn is followed by another mixed flow reactor, 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. 6.12. This allows us to predict the overall conversions for such systems, or conversions at intermediate points between the individual reactors. These intermediate conversions may be needed to determine the duty of interstage heat exchangers.

Best Arrangement of a Set of Ideal Reactors. For the most effective use of a given set of ideal reactors we have the following general rules:

1. For a reaction whose rate-concentration curve rises monotonically (any n th-order reaction, $n > 0$) 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 ($n > 1$), and as low as possible if the curve is convex ($n < 1$). As an example, for the case of Fig. 6.12 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.

The problems at the end of this chapter illustrate these findings.