University of Anbar

College of Engineering

Chemical and Petrochemical Engineering Department

Chemical Reacior Design

Third Year

Dr. Suha Akram

Lecture No. 10

SIZE COMPARISON OF SINGLE REACTORS

Mixed Versus Plug Flow Reactors, First- and Second-Order Reactions:

The **ratio of sizes** of mixed and plug flow reactors will depend on the **extent of reaction, the stoichiometry, and the form of the rate equation.**

For the general case ,a comparison of Eqs. 5.11 and 5.17 will give this size ratio. Let us make this comparison for the large class of reactions approximated by the simple ***nth***-order rate law

$$-r_A = -\frac{1}{V}\frac{dN_A}{dt} = kC_A^n$$

where n varies anywhere from zero to three. For mixed flow Eq. 5.11 gives

$$\tau_m = \left(\frac{C_{A0}V}{F_{A0}}\right)_m = \frac{C_{A0}X_A}{-r_A} = \frac{1}{kC_{A0}^{n-1}}\frac{X_A(1+\varepsilon_A X_A)^n}{(1-X_A)^n}$$

whereas for plug flow Eq. 5.17 gives

$$\tau_p = \left(\frac{C_{A0}V}{F_{A0}}\right)_p = C_{A0}\int_0^{X_A}\frac{dX_A}{-r_A} = \frac{1}{kC_{A0}^{n-1}}\int_0^{X_A}\frac{(1+\varepsilon_A X_A)^n dX_A}{(1-X_A)^n}$$

Dividing we find that

$$\frac{(\tau C_{A0}^{n-1})_m}{(\tau C_{A0}^{n-1})_p} = \frac{\left(\frac{C_{A0}^n V}{F_{A0}}\right)_m}{\left(\frac{C_{A0}^n V}{F_{A0}}\right)_p} = \frac{\left[X_A\left(\frac{1+\varepsilon_A X_A}{1-X_A}\right)^n\right]_m}{\left[\int_0^{X_A}\left(\frac{1+\varepsilon_A X_A}{1-X_A}\right)^n dX_A\right]_p} \qquad \textbf{(1)}$$

With constant density, or $\varepsilon = 0$, this expression integrates to

$$\frac{(\tau C_{A0}^{n-1})_m}{(\tau C_{A0}^{n-1})_p} = \frac{\left[\frac{X_A}{(1-X_A)^n}\right]_m}{\left[\frac{(1-X_A)^{1-n}-1}{n-1}\right]_p}, \qquad n \neq 1$$

or **(2)**

$$\frac{(\tau C_{A0}^{n-1})_m}{(\tau C_{A0}^{n-1})_p} = \frac{\left(\frac{X_A}{1-X_A}\right)_m}{-\ln(1-X_A)_p}, \qquad n = 1$$

Equations 1 and 2 are displayed in graphical form in Fig. 6.1 to provide a quick comparison of the performance of plug flow with mixed flow reactors. For

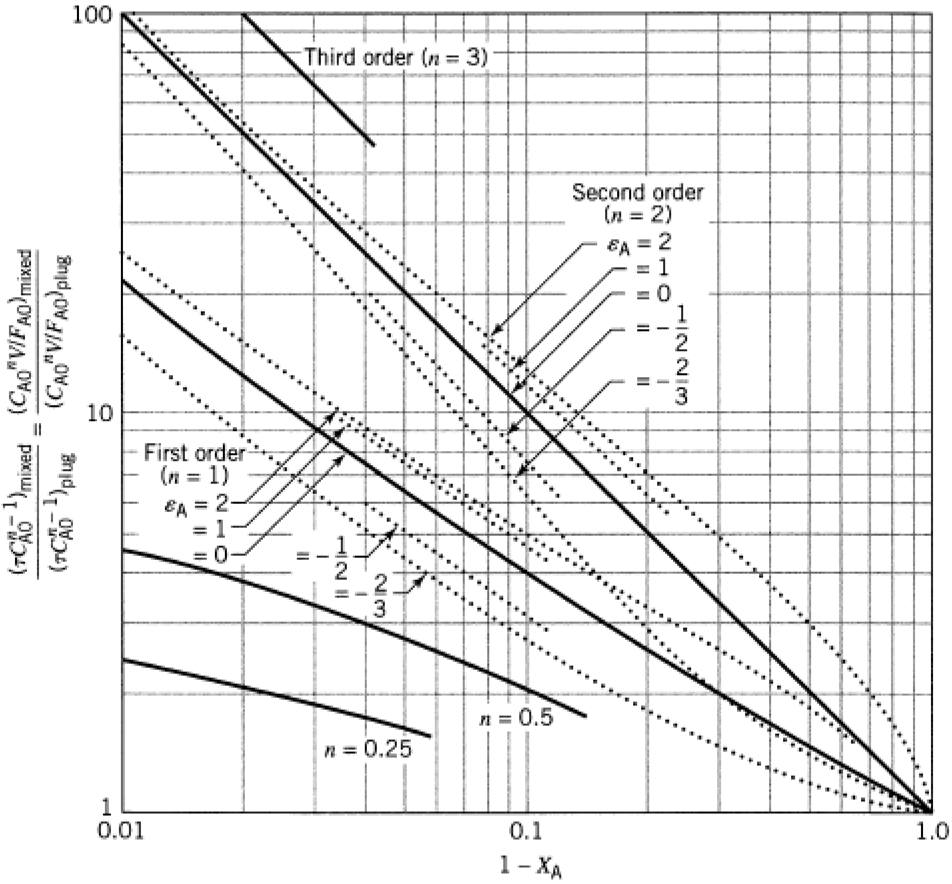

Figure 6.1 Comparison of performance of single mixed flow and plug flow reactors for the nth-order reactions

$$A \rightarrow \text{products}, \quad -r_A = kC_A^n$$

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.

identical feed composition C_{A0} and flow rate F_{A0} the ordinate of this figure gives directly the volume ratio required for any specified conversion. Figure 6.1 shows the following.

1. For any particular duty and for all positive reaction orders the mixed reactor is always larger than the plug flow reactor. The ratio of volumes increases with reaction order.
2. 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.
3. Density variation during reaction affects design; however, it is normally of secondary importance compared to the difference in flow type.

Variation of Reactant Ratio for Second-Order Reactions

Second-order reactions of two components and of the type

$$A + B \rightarrow \text{products}, \qquad M = C_{B0}/C_{A0}$$
$$-r_A = -r_B = kC_AC_B \qquad \textbf{(3.13)}$$

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

$$-r_A = kC_AC_B = kC_A^2 \qquad \text{when } M = 1 \qquad \textbf{(3)}$$

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

$$-r_A = kC_AC_B = (kC_{B0})C_A = k'C_A \qquad \text{when } M \gg 1 \qquad \textbf{(4)}$$

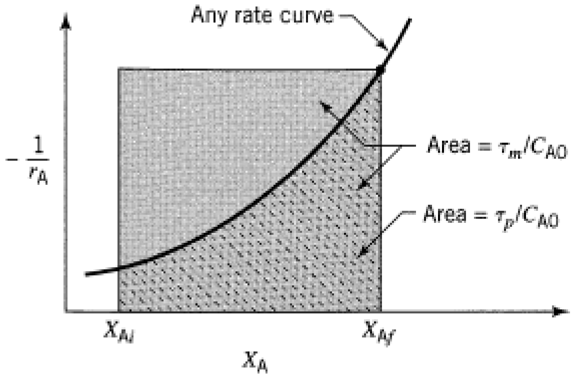

Figure 6.2 Comparison of performance of mixed flow and plug flow reactors for any reaction kinetics.

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 nth-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 $X_1, X_2, \ldots, X_N$ be the fractional conversion of component A leaving reactor $1, 2, \ldots, N$. Basing the material balance on the feed rate of A to the first reactor, we find for the ith 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

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

$$= \int_{X_0=0}^{X_1} \frac{dX}{-r} + \int_{X_1}^{X_2} \frac{dX}{-r} + \cdots + \int_{X_{N-1}}^{X_N} \frac{dX}{-r} = \int_0^{X_N} \frac{dX}{-r}$$

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.

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?

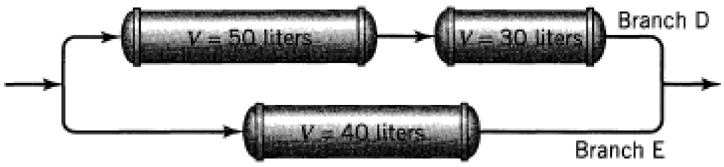

Figure E6.1

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,

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

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

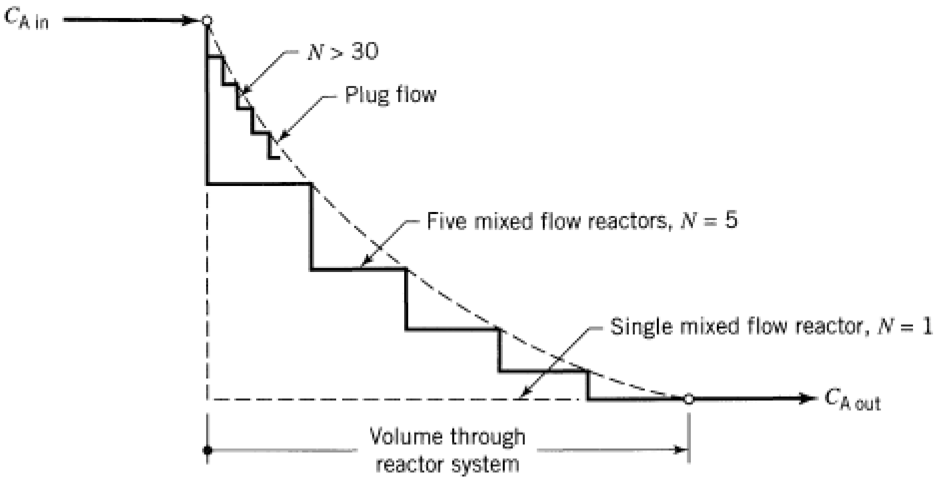

Figure 6.3 Concentration profile through an *N*-stage mixed flow reactor system compared with single flow reactors.

Equal-Size Mixed Flow Reactors in Series:

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.

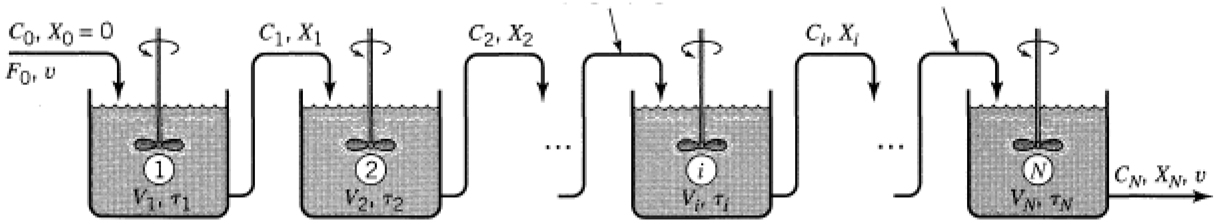

Figure 6.4 Notation for a system of *N* equal-size mixed reactors in series.

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

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

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

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

Rearranging, we find for the system as a whole

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

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

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

With Eqs. 6*b* and 7 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.

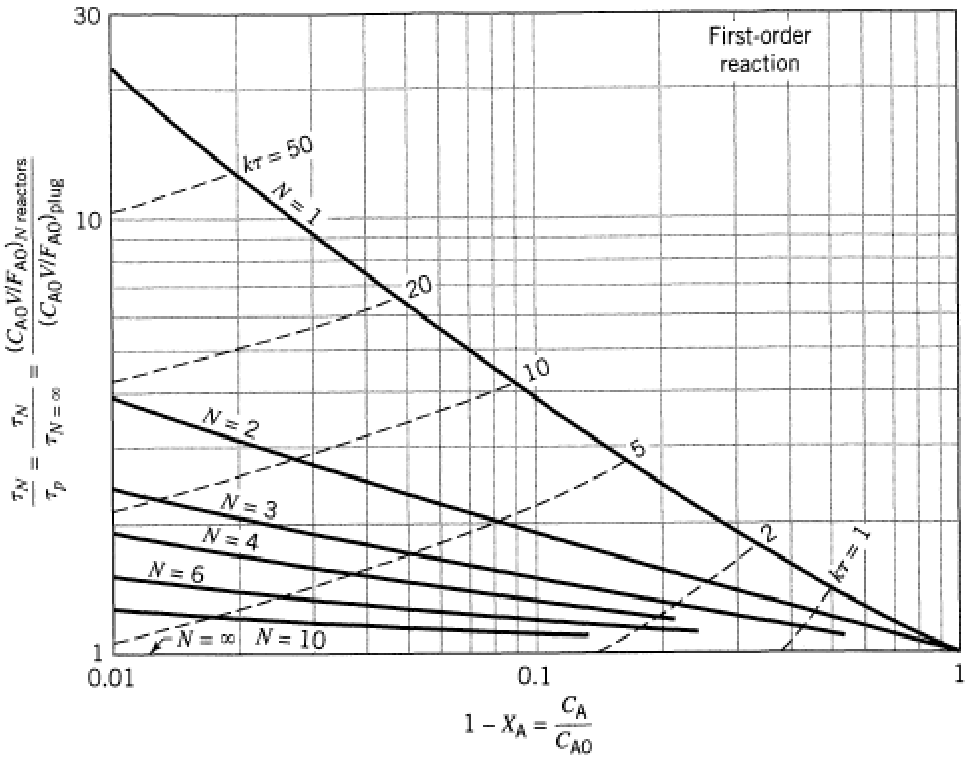

Figure 6.5 Comparison of performance of a series of N equal-size mixed flow reactors with a plug flow reactor for the first-order reaction

Second-Order Reactions. : 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

$A \rightarrow R, \qquad \varepsilon = 0$

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

$$C_N = \frac{1}{4k\tau_i}\left(-2 + 2\sqrt{\underbrace{-1 \cdots + 2\sqrt{-1 + 2\sqrt{1 + 4C_0k\tau_i}}}_{\vdots}}\right\}N\Bigg) \qquad \textbf{(8a)}$$

whereas for plug flow

$$\frac{C_0}{C} = 1 + C_0k\tau_p \qquad \textbf{(8b)}$$

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

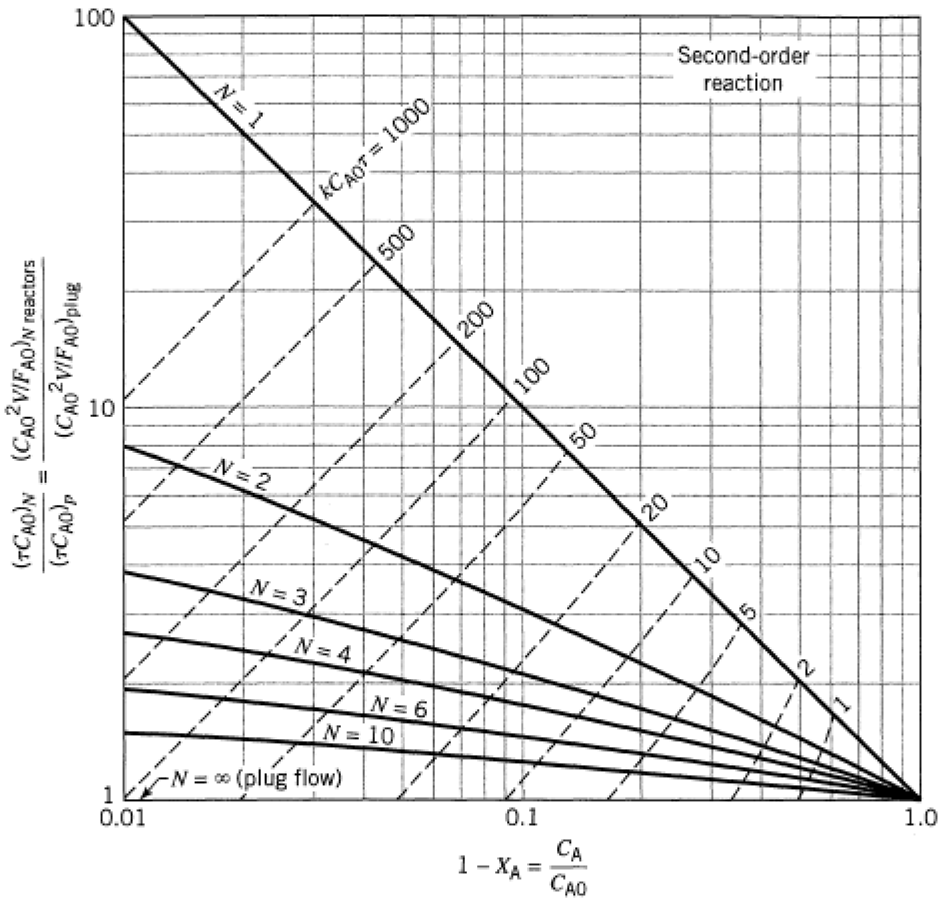

Figure 6.6 Comparison of performance of a series of N equal-size mixed flow reactors with a plug flow reactor for elementary second-order reactions

$2A \rightarrow$ products

$A + B \rightarrow$ products, $\quad C_{A0} = C_{B0}$

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.