## UNIT-3

## DESIGN OF MULTIPLE REACTORS FOR SINGLE REACTIONS

## INTRODUCTION

There are many ways of processing a fluid: in a single batch or flow reactor, in a chain of reactors possibly with interstage feed injection or heating and in a reactor with recycle of the product stream using various feed ratios and conditions. The reactor system selected will influence the economics of the process by dictating the size of the units needed and by 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. For single reactions product distribution is fixed; hence, the important factor in comparing designs is the reactor size. The size comparison of various single and multiple ideal reactor systems is considered.

## SIZE COMPARISON OF SINGLE REACTORS

## Batch Reactor

The batch reactor has the advantage of small instrumentation cost and flexibility of operation (may be shut down easily and quickly). It has the disadvantage of high labor and handling cost, often considerable shutdown time to empty, clean out, and refill, and poorer quality control of the product. Hence it may be generalized to state that the batch reactor is well suited to produce small amounts of material and to produce many different products from one piece of equipment. On the other hand, for the chemical treatment of materials in large amounts the continuous process is nearly always found to be more economical.

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

For a given duty 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.

$$
-r_{A}=-1 d N_{A}
$$

$$
-\cdots------=\mathrm{kC}_{\mathrm{A}}{ }^{\mathrm{n}}
$$

V dt
$\left(\tau \mathrm{C}_{\mathrm{AO}}{ }^{\mathrm{n}-1}\right) \mathrm{m} /\left(\tau \mathrm{C}_{\mathrm{AO}}{ }^{\mathrm{n}-1}\right) \mathrm{m}$
Is represented by the following graph


To provide a quick comparison of the performance of plug flow with mixed flow reactors, the performance graph is used. For identical feed composition $C A o$ and flow rate $F A$, the ordinate of this figure gives directly the volume ratio required for any specified conversion.

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. Dashed lines represent fixed values of the dimensionless reaction rate group, defined as
$\boldsymbol{k} \boldsymbol{\tau}$ for first-order reaction
$\boldsymbol{k} \boldsymbol{C}_{\boldsymbol{A} \boldsymbol{0}} \boldsymbol{\tau}$ for second-order reaction
With these lines we can compare different reactor types, reactor sizes, and conversion levels.
Second-order reactions of two components and of the type behave as second-order reactions of one component when the reactant ratio is unity. Thus
$-r A=k C A C B=k c ;$ when $M=1$
On the other hand, when a large excess of reactant $B$ is used then its concentration does not change appreciably $(C B=C B O)$ and the reaction approaches first-order behavior with respect to the limiting component $\mathbf{A}$, or
$-r A=k C A C B=(k C B O) C=A k r C A$ when $\mathrm{M}+1$
Thus terms of the limiting component A , the size ratio of mixed to plug flow reactors is represented by the region between the first-order and the second-order curves.


For reactions with arbitrary but known rate the performance capabilities of mixed and plug flow reactors are best illustrated in above figure. The ratio of shaded and of hatched areas gives the ratio of space-times needed in these two reactors. The rate curve drawn in above figure is typical of the large class of reactions whose rate decreases continually on approach to equilibrium (this includes all nth-order reactions, $\mathrm{n}>0$ ). For such reactions it can be seen that mixed flow always needs a larger volume than does plug flow for any given duty.

## Plug Flow Reactors in Series and / or in Parallel

Consider N plug flow reactors connected in series, and let $\mathrm{X}_{1}, \mathrm{X}_{2}, \ldots, \mathrm{X}_{\mathrm{N}}$, 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
$\mathrm{V}_{\mathrm{i}} / \mathrm{F}_{\mathrm{O}}=\tau_{\mathrm{i}} / \mathrm{C}_{\mathrm{AO}}=\int \mathrm{dX} /(-\mathrm{r})$
or for the N reactors in series
$\mathrm{V} / \mathrm{F}_{\mathrm{O}}=\Sigma \mathrm{Vi} / \mathrm{F}_{\mathrm{O}}=\int \mathrm{dX} /\left(-\mathrm{r}_{)}\right.$

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 .

## OPERATING A NUMBER OF PLUG FLOW REACTORS

The reactor setup shown in Figure 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?


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

## 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 nth-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 above figure, 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. Quantitatively evaluate the behavior of a series of N equal-size mixed flow reactors. Density changes will be assumed to be negligible; hence $\boldsymbol{\rho}=0$. As a rule, with mixed flow reactors it is more convenient to develop the necessary equations in terms of concentrations rather than fractional conversions .

## Problems using Comparison Charts

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 theone being used in series with it.
(a) For the same treatment rate as that used at present, how will this additionaffect the conversion of reactant?
(b) For the same $90 \%$ conversion, by how much can the treatment rate be increased?


(a) Find the conversion for the same treatment rate. For the single reactor at $90 \%$ conversion we have from chart
$k C o \tau=90$
For the two reactors the space-time or holding time is doubled; hence, the operation will be represented by the dashed line of chart where
$k \operatorname{Co\tau }=180$
This line cuts the $\mathrm{N}=2$ line at a conversion $\mathrm{X}=97.4 \%$, point a .
(b) Find the treatment rate for the same conversion. Staying on the $90 \%$ conversion
line, we find for $\mathrm{N}=2$ that
$k C o \tau=27.5$, point b
Comparing the value of the reaction rate group for $\mathrm{N}=1$ and $\mathrm{N}=2$, we find
Since $V_{2}=2 V_{1}$ the ratio of flow rates becomes
Thus, the treatment rate can be raised to 6.6 times the original.


## 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.

## 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 $\boldsymbol{r}$ versus C curve for component A to represent the reaction rate at various concentrations. It is illustrated by 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 $\boldsymbol{\rho}=\mathrm{O}$ ), and volumetric flow rates as shown in figure below. Now from equation noting that $\boldsymbol{\rho}=0$, we may write for component $\mathbf{A}$ in the first reactor


$$
\begin{aligned}
& \tau_{1}=V_{1} / V=C_{0} \cdot C_{1} /\left(-r_{1}\right) \\
& -1 / \tau_{1}=\left(\cdot r_{1}\right) / C_{1} \cdot C_{0} \\
& \text { For ith reactor } \\
& -1 / \tau_{i}=\left(\cdot r_{i}\right) / C_{i} \cdot C_{i-1}
\end{aligned}
$$



Plot the C versus r curve for component A and it is as shown in figure above. To find the conditions in the first reactor note that the inlet concentration Co is known (point L ), that C , and $(-\boldsymbol{r})$, correspond to a point on the curve to be found (point M), and that the slope of the line $\mathrm{LM}=\mathrm{MNINL}=(-\mathrm{r}), 1(\mathrm{C},-\mathrm{Co})=-(1 / \mathrm{rl})$ from equation. Hence, from Co draw a line of slope ( $1 / \mathrm{r}$, ) until it cuts the rate curve; this gives C1. Similarly, we find from equation, that a line of slope $-(1 / \mathrm{r} 2)$ 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

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 following procedure is followed. The basic performance expressions, from equations, give, in turn, for the first reactor

$\tau_{1 /} C_{0}=X_{1} /\left(\cdot r_{1}\right)$
and for the second reactor
$\tau_{2}, C_{0}=X_{2} \cdot X_{1} /\left(-r_{2}\right)$
as the intermediate conversion $X I$ 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 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 XI (or point M on the curve) so as to maximize the area of this rectangle. This is done according to Maximization of Rectangles concept.In the below figure, construct a rectangle between the $x-y$ axes and touching the arbitrary curve at point $\mathrm{M}(\mathrm{x}, \mathrm{y})$. The area of the rectangle is then
$A=x y$
This area is maximized when
$\mathrm{da}=0=\mathrm{xdy}+\mathrm{ydx}$
or when $-d y / d x=y / x$


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 nth-order kinetics, $\mathrm{n}>0$, there always is just one "best" point. 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 figure, and this determines the intermediate conversion $X$, 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 $\mathrm{n}<1$ the larger should come first. 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.

## 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 nth-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 ( $n>\mathrm{I}$ ), and as low as possible if the curve is convex $(\mathrm{n}<1)$. As an example, for the case of above figure 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 $1 /(-\mathrm{r})$ vs. CA curve is a good way to find the best arrangement of units.
