Design for Single Reactions

Chapter 6

Design for Single Reactions

There are many ways of processing a fluid:

- Single batch or flow reactor.
- Chain of reactors possibly with inter stage feed injection or heating.
- Reactor with recycle of the product stream using various feed ratios and conditions.
- Which scheme should we use? Unfortunately, numerous factors may have to be considered in answering this question
- In this chapter we deal with single reactions.

SIZE COMPARISON OF SINGLE REACTORS Batch Reactor

- 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.
- Batch reactor is well suited to produce small amounts of material and to produce many different products from one piece of equipment.
- It is easy to relate the performance capabilities of the batch reactor with the plug flow reactor.

Mixed Versus Plug Flow Reactors, Firstand Second-Order Reactions

 comparison for the large class of reactions approximated by the simple nth-order rate law

$$-r_{\rm A} = -\frac{1}{V} \frac{dN_{\rm A}}{dt} = kC_{\rm A}^{n}$$

$$\tau_{m} = \left(\frac{C_{\rm A0}V}{F_{\rm A0}}\right)_{m} = \frac{C_{\rm A0}X_{\rm A}}{-r_{\rm A}} = \frac{1}{kC_{\rm A0}^{n-1}} \frac{X_{\rm A}(1+\varepsilon_{\rm A}X_{\rm A})^{n}}{(1-X_{\rm A})^{n}}$$

$$\tau_{p} = \left(\frac{C_{\rm A0}V}{F_{\rm A0}}\right)_{p} = C_{\rm A0} \int_{0}^{X_{\rm A}} \frac{dX_{\rm A}}{-r_{\rm A}} = \frac{1}{kC_{\rm A0}^{n-1}} \int_{0}^{X_{\rm A}} \frac{(1+\varepsilon_{\rm A}X_{\rm A})^{n} dX_{\rm A}}{(1-X_{\rm A})^{n}}$$

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

Comparison for nth-order rate law

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

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

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

Comparison of the performance of plug flow with mixed flow reactors



Comparison of the performance of plug flow with mixed flow reactors

- The ordinate becomes the volume ratio V_m/V_p or spacetime ratio T_m/T_p if the same quantities of identical feed are used.
- Identical feed composition C_{Ao} and flow rate F_{Ao} 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
- **3.** Density variation during reaction affects design; however, it is normally of secondary importance compared to the difference in flow type.
- **4.** In plug flow, the concentration of reactant decreases progressively through the system;
- **5.** In mixed flow, the concentration drops immediately to a low value.
- 6. 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.

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



Includes all nth-order reactions, n > 0

- The ratio of shaded and of hatched areas gives the ratio of space-times needed in these two reactors.
- Mixed flow always needs a larger volume than does plug flow for any given duty.

MULTIPLE-REACTOR SYSTEMS

Plug Flow Reactors in Series and/or in Parallel

N plug flow reactors connected in series, and let X_1, X_2, \ldots, X_n be fractional conversion of component A leaving reactor 1, 2, ..., N.

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

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

Branch D consists of two reactors in series; hence, it may be considered to be a single reactor of volume

 $V_{\rm D} = 50 + 30 = 80$ liters

Now for reactors in parallel V/F must be identical if the conversion is to be the same in each branch. Therefore,

$$\left(\frac{V}{F}\right)_{\rm D} = \left(\frac{V}{F}\right)_{\rm E} \qquad \qquad \frac{F_{\rm D}}{\underline{F_{\rm E}}} = \frac{V_{\rm D}}{V_{\rm E}} = \frac{80}{40} = \underline{\underline{2}}$$

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

Equal-Size Mixed Flow Reactors in Series



First-Order Reactions

Material balance for component A about vessel i

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

For
$$\varepsilon = 0$$

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

Space-time τ (or mean residence time t) is the same in all the equal size reactors of volume *Vi*.

Therefore

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

Total τ for N reactor

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

For N $\rightarrow \mathbb{R}$, this equation reduces to the plug flow equation

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

Comparison of series of *N* equal-size mixed flow with plug flow reactor (first-order reaction)



Second-Order Reactions

• N reactors in series we find

$$C_{N} = \frac{1}{4k\tau_{i}} \left(-2 + 2\sqrt{\frac{1}{-1\cdots+2\sqrt{-1+2\sqrt{1+4C_{0}k\tau_{i}}}}} \right)$$

• Whereas for plug flow

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





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.

- (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?



(a) Find the conversion for the same treatment rate.

For the single reactor at 90% conversion we have $kCo\tau = 90$.

For the two reactors the space-time or holding time is doubled; $kCo \tau = 180$

Staying on the 90% conversion line, we find for N = 2 that $kCo \tau$ = 27.5

 Comparing the value of the reaction rate group for N = 1 and N = 2, we

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

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.

Mixed Flow Reactors of Different Sizes in Series

Two types of questions may be asked:

- how to find the outlet conversion from a given reactor system,
- Inverse question, how to find the best setup to achieve a given conversion.

Finding the Conversion in a Given System

considering three mixed flow reactors in series with volumes, feed rates, concentrations, space-times, volumetric flow rates

• space-times equal to residence times because $\epsilon = 0$

Notation for a series of unequal-size mixed flow reactors



Volumetric flow rates is same at steady state

$$\tau_1 = \overline{t}_1 = \frac{V_1}{v} = \frac{C_0 - C_1}{(-r)_1}$$
$$-\frac{1}{\tau_1} = \frac{(-r)_1}{C_1 - C_0}$$



Determining the Best System (Given Conversion)



Maximization of Rectangles

construct a rectangle between the x-y axes and touching the arbitrary curve at point M(x, y). The area of the rectangle is the



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, n > 0, there always is just one "best" point

Optimum size ratio of the two reactors

Slope of the rate curve at M equals the diagonal NL.

This determines the intermediate conversion X_1 as well as the size of units needed.



Reactors of Different Types in Series



Performance equation the three reactors

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

Guidelines for order of reactors nth-order reaction,

- n > 0 Reactors should be connected in series
- n > I Keep the concentration of reactant as high as possible
- n < 1 As low as possible if the curve is convex

RECYCLE REACTOR

Advantageous to divide the product stream from a plug flow reactor and return a portion of it to the entrance of the reactor.

Let the *recycle ratio* R

 $\mathbf{R} = \frac{\text{volume of fluid returned to the reactor entrance}}{\text{volume leaving the system}}$

 Recycle ratio is raised the behavior shifts from plug flow (R = 0) to mixed flow (R = 2).



$$\frac{V}{F'_{A0}} = \int_{X_{A1}}^{X_{A2}=X_{Af}} \frac{dX_{A}}{-r_{A}}$$

RECYCLE REACTOR

Where F_{Ao} would be the feed rate of A if the stream entering the reactor (fresh feed plus recycle) were unconverted

 $F'_{A0} = \begin{pmatrix} A \text{ which would enter in an} \\ \text{unconverted recycle stream} \end{pmatrix} + \begin{pmatrix} A \text{ entering in} \\ \text{fresh feed} \end{pmatrix}$

$$= \mathbf{R}F_{A0} + F_{A0} = (\mathbf{R} + 1)F_{A0}$$

$$X_{A1} = \frac{1 - C_{A1}/C_{A0}}{1 + \varepsilon_{A}C_{A1}/C_{A0}} \qquad C_{A1} = \frac{F_{A1}}{v_{1}} = \frac{F_{A0} + F_{A3}}{v_{0} + Rv_{f}}$$
$$X_{A1} = \left(\frac{R}{R+1}\right) X_{Af} \qquad C_{A1} = \frac{F_{A1}}{v_{1}} = \frac{F_{A0} + F_{A3}}{v_{0} + Rv_{f}}$$
$$C_{A1} = \frac{F_{A1}}{v_{1}} = \frac{F_{A1}}{v_{0} + Rv_{f}}$$
$$C_{A1} = \frac{F_{A1}}{v_{0} + Rv_{f}}$$

XI = 1 - Gal/Gao
14 En Gal/Gao
At point (C) Stream meeting at point (R) may be
added directly.
for finiting (in or x) Gal = FAI = Front FAZ =

$$v_1 = \frac{FAI}{v_1} = \frac{FAI}{v_0 + R v_1}$$

for finiting (in or x) Gal = Caller (1+R - R Mar)
Rvf = Rvo(1+ Cinx AJ (Gal = Gao (1+R - R Mar)
Rvf = Rvo(1+ Cinx AJ) (Gal = Gao (1+R - R Mar)

CHAPMO. FAO r, Vo. FA3 CER FAD RYC (Br Vi= NotRyf MJ-XGIIERXAJ) but hear feed is to not fresh bo. FA3 - FAO (1 - XAJ)

$$f_{A_1} = F_{A_0} + f_{A_3}$$

$$= f_{A_0} + R_{F_{A_0}} + (1 - x_4)$$

$$f_{A_1} = F_{A_0} + (1 + R - Rx_4)$$

$$f_{A_1} = \frac{f_{A_0} + (1 + R - Rx_4)}{y_0 + y_0 + y_0}$$

$$\chi_1 = \frac{1 - \frac{G_{A_1}}{G_{A_0}}}{1 + \frac{G_{A_1}}{G_{A_0}}}$$

$$\chi_1 = \frac{1 - \frac{G_{A_1}}{G_{A_0}}}{1 + \frac{G_{A_1}}{G_{A_0}}}$$

$$\chi_1 = \frac{1 - \frac{(1 + R - Rx_4)}{G_{A_0}}}{1 + \frac{G_{A_1}}{G_{A_0}}}$$

$$= \frac{\left(\frac{1}{1+R} + R \operatorname{Cn}_{2} \operatorname{kf} - \sqrt{-R + R \operatorname{mn}_{f}}\right)}{1 + R + R \operatorname{Cn}_{2} \operatorname{kf}_{f}}$$

$$= \frac{1}{1+R + R \operatorname{Cn}_{2} \operatorname{kf}_{f}} + \frac{1}{1+R + R \operatorname{Cn}_{2} \operatorname{kf}_{f}}$$

$$= \frac{1}{1+R + R \operatorname{Cn}_{f}} + \frac{1}{1+R + R \operatorname{Cn}_{f}}$$

$$= \frac{1}{1+R + R \operatorname{Cn}_{f}} + \frac{1}{1+R + R \operatorname{Cn}_{f}}$$

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$$= \frac{1}{1+R + R \operatorname{Cn}_{f}} + \frac{1}{1+R + R \operatorname{Cn}_{f}}$$

terms of GA. for GA-0

$$\frac{N}{FAD} = (RAD) \int_{-\infty}^{\infty} \frac{1}{P} \frac{dx}{P} \frac{dx$$

In

RECYCLE REACTOR

• Performance equation for recycle reactors,

good for any kinetics, any ε value and for $X_A = 0$



The approach to these extremes



 $\frac{k\tau}{\boldsymbol{R}+1} = \ln\left[\frac{C_{A0} + \boldsymbol{R}C_{Af}}{(\boldsymbol{R}+1)C_{Af}}\right]$

Integration of the recycle equation gives, for *first-order reaction*, $\varepsilon = 0$,





first-order reactions



Comparison of performance of recycle and plug flow for first-order reactions



Comparison of performance of recycle reactors with plug flow reactors (second-order reactions)

AUTOCATALYTIC REACTIONS

 $A + R \rightarrow R + R$, $-r_A = kC_A^a C_R^r$

- Reactions with such rate-concentration curves lead to interesting optimization problems
- $1/(-r_A)$ versus X_A curves with their characteristic minima

Plug Flow Vs Mixed Flow Reactor (No Recycle)

Which reactor is superior for a given job (which requires a smaller volume)

- **1.** At low conversion the mixed reactor is superior to the plug flow reactor.
- 2. At high enough conversions the plug flow reactor is superior.
- we should note that a plug flow reactor will not operate at all with a feed of pure reactant.
- In such a situation the feed must be continually primed with product, an ideal opportunity for using a recycle reactor.

Optimum Recycle Operations

- When material is to be processed to some fixed final conversion X_{Af} in a recycle reactor.
- A particular recycle ratio which is optimum in that it minimizes the reactor volume or space-time.
- The optimum recycle ratio is found by differentiating with respect to R and setting to zero.

$$\frac{d(\tau/C_{A0})}{d\mathbf{R}} = 0 \qquad \frac{\tau}{C_{A0}} = \int_{X_{Af}}^{X_{Af}} \frac{\mathbf{R} + 1}{(-r_{A})} dX_{A}$$

• From the theorems of calculus, if

$$F(\boldsymbol{R}) = \int_{a(\boldsymbol{R})}^{b(\boldsymbol{R})} f(x, \boldsymbol{R}) \, dx$$

$$\frac{dF}{d\mathbf{R}} = \int_{a(\mathbf{R})}^{b(\mathbf{R})} \frac{\partial f(x,\mathbf{R})}{\partial \mathbf{R}} dx + f(\mathbf{b},\mathbf{R}) \frac{db}{d\mathbf{R}} - f(a,\mathbf{R}) \frac{da}{d\mathbf{R}}$$

$$\frac{d(\tau/C_{A0})}{d\mathbf{R}} = 0 = \int_{X_{Ai}}^{X_{Af}} \frac{dX_A}{(-r_A)} + 0 - \frac{\mathbf{R}+1}{(-r_A)} \bigg|_{X_{Ai}} \frac{dX_{Ai}}{d\mathbf{R}}$$

$$\frac{dX_{\mathrm{A}i}}{d\boldsymbol{R}} = \frac{X_{\mathrm{A}f}}{(\boldsymbol{R}+1)^2}$$

$$\frac{T}{AB} = \int_{1}^{N_{f}} (R+n) \frac{dn}{dn} = \frac{1}{2} \int_{1}^{N_{f}} F(R) = \int_{0}^{D} f(n,R) dn = \frac{1}{2} \int_{0}^{N_{f}} f(n,R) dn = \frac{1}{2} \int_{0}^{D} \frac{dr}{dR} = \int_{0}^{D} \frac{df(n,R)}{dR} dn = \frac{1}{2} \int_{0}^{D} \frac{dr}{dR} = \int_{0}^{D} \frac{df(n,R)}{dR} dn + \frac{1}{2} \int_{0}^{D} \frac{dr}{dR} = \int_{0}^{D} \frac{dr}{dR} dn + \frac{1}{2} \int_{0}^{D} \frac{dr}{dR} = \int_{0}^{D} \frac{dr}{dR} dn + \frac{1}{2} \int_{$$

MAI - RAM (may - nai) - R may. (Reis Real - Romang-267

In words, the optimum recycle ratio introduces to the reactor a feed whose $l/(-r_A)$ value (KL) equals the average ll(-rA) value in the reactor as a whole (PQ in Fig. 6.20).

Occurrence of Autocatalytic Reactions.

- The most important examples of autocatalytic reactions are the broad class of fermentation reactions which result from the reaction of microorganism on an organic feed.
- Another type of reaction which has autocatalytic behavior is the exothermic reaction (say, the combustion of fuel gas)
- *Autothermal,* heat may be considered to be the product which sustains the reaction.

Reactor Combinations

- For autocatalytic reactions all sorts of reactor arrangements are to be considered
- if product recycle or product separation with recycle is allowable
- one should always try to reach point M in one step (using mixed flow in a single reactor)
- Then follow with plug flow or as close to plug flow as possible.

When separation and reuse of unconverted reactant is possible, operate at point M

FINDING THE BEST REACTOR SETUP

 At a given enzyme concentration C_E tests in a laboratory mixed flow reactor give the following results:

C_{A0} , mmol/m ³	2	5	6	6	11	14	16	24
$C_{\rm A}$, mmol/m ³	0.5	3	1	2	6	10	8	4
τ , min	30	1	50	8	4	20	20	4

We wish to treat 0.1 m³/min of this waste water having $C_{A0} = 10 \text{ mmol/m}^3$ to 90% conversion with this enzyme at concentration C_E .

(a) One possibility is to use a long tubular reactor (assume plug flow) with possible recycle of exit fluid. What design do you recommend? Give the size of the reactor, tell if it should be used with recycle, and if so determine the recycle flow rate in cubic meters per minute (m³/min). Sketch your recommended design.

Solution

oración	C_{A0} , mmol/m ³	2	5	6	6	11	14	16	24
	$C_{\rm A}$, mmol/m ³	0.5	3	1	2	6	10	8	4
	τ , min	30	1	50	8	4	20	20	4
$\frac{1}{-r_{\rm A}} = \frac{1}{C_{\rm A0}}$	$\frac{\tau}{-C_{\rm A}}, \frac{{\rm m}^3 \cdot {\rm min}}{{\rm mmol}}$	20	0.5	10	2	0.8	5	2.5	0.2

Part (a) Solution. From the $-1/r_A$ vs. C_A curve we see that we should use plug flow with recycle.

(b) Another possibility is to use one or two stirred tanks (assume ideal). What two-tank design do you recommend, and how much better is it than the one-tank arrangement?

Part (b) Solution.

Drawing slopes and diagonals according to the method of maximization of rectangles

(c) What arrangement of plug flow and mixed flow reactors would you use to minimize the total volume of reactors needed? Sketch your recommended design and show the size of units selected. We should mention that separation and recycle of part of the product stream is not allowed.

Part (c) Solution.

Following the reasoning in this chapter we should use a mixed flow reactor followed by a plug flow reactor.

6.1. A liquid reactant stream (1 mol/liter) passes through two mixed flow reactors in a series. The concentration of A in the exit of the first reactor is 0.5 mol/liter. Find the concentration in the exit stream of the second reactor. The reaction is second-order with respect to A and $V_2/V_1 = 2$.

6.1 For a second order reaction:
$$kT = \frac{C_{AD} - C_A}{C_A^2}$$
, so for the two reactors

$$\frac{V_2}{V_1} = 2 = \frac{kT_2}{kT_1} = \frac{(C_{A1} - C_{A2})/c_{A2}^2}{(C_{A0} - C_{A1})/c_{A1}^2} = \frac{(0.5 - C_{A2})/c_{A2}^2}{(1 - 0.5)/0.5^2}$$
or
 $4C_{A2}^2 = 0.5 - C_{A2}$
therefore
 $C_{A2} = 0.25 \text{ mol}/Lit$.

6.3. An aqueous reactant stream (4 mol A/liter) passes through a mixed flow reactor followed by a plug flow reactor. Find the concentration at the exit of the plug flow reactor if in the mixed flow reactor $C_A = 1$ mol/liter. The reaction is second-order with respect to A, and the volume of the plug flow unit is three times that of the mixed flow unit.

6.3 For the second order reaction
for the mixed flow reactor:
$$k_{1}T_{m} = \frac{C_{A0}-C_{A1}}{C_{A1}^{2}} = \frac{4-1}{1} = 3$$

so for the plug flow reactor: $k_{1}T_{m} = \frac{C_{A0}-C_{A1}}{C_{A1}^{2}} = \frac{4-1}{1} = 3$
and $\frac{C_{A2}}{C_{A1}} = \frac{1}{1+k_{1}T_{p}C_{A1}} = \frac{1}{1+q_{1}C_{1}} = 0.1$
 $\therefore C_{A2} = 0.1 (C_{A1}) = 0.1 \text{ mol/lit}$

6.5. Originally we had planned to lower the activity of a gas stream containing radioactive Xe-138 (half-life = 14 min) by having it pass through two holdup tanks in series, both well mixed and of such size that the mean residence time of gas is 2 weeks in each tank. It has been suggested that we replace the two tanks with a long tube (assume plug flow). What must be the size of this tube compared to the two original stirred tanks, and what should be the mean residence time of gas in this tube for the same extent of radioactive decay?

6.7. We wish to treat 10 liters/min of liquid feed containing 1 mol A/liter to 99% conversion. The stoichiometry and kinetics of the reaction are given by

$$A \rightarrow R$$
, $-r_A = \frac{C_A}{0.2 + C_A} \frac{\text{mol}}{\text{liter} \cdot \text{min}}$

Suggest a good arrangement for doing this using two mixed flow reactors, and find the size of the two units needed. Sketch the final design chosen.

6.9. At present we have 90% conversion of a liquid feed $(n = 1, C_{A0} = 10 \text{ mol/} \text{liter})$ to our plug flow reactor with recycle of product $(\mathbf{R} = 2)$. If we shut off the recycle stream, by how much will this lower the processing rate of our feed to the same 90% conversion?

6.9 With recycle for a first order reaction we have

$$kT = (R+1) ln \left[\frac{C_{AD} + RC_{AF}}{(R+1)C_{AF}} \right] = (2+1) ln \left[\frac{10+2(1)}{(2+1)1} \right] = 3 ln 4$$
Without recycle (plug flow)

$$kT = ln \frac{C_{AD}}{C_{AF}} = ln 10$$
Therefore

$$\frac{U_{without}}{U_{with}} = \frac{T_{with}}{T_{withat}} = \frac{3 ln 4}{ln 10} = 1.8$$

6.11. Consider the autocatalytic reaction $A \rightarrow R$, with $-r_A = 0.001 C_A C_R \text{ mol/}$ liter \cdot s. We wish to process 1.5 liters/s of a $C_{A0} = 10$ mol/liter feed to the highest conversion possible in the reactor system consisting of four 100liter mixed flow reactors connected as you wish and any feed arrangement. Sketch your recommended design and feed arrangement and determine C_{Af} from this system.

6.11 For this autocatalytic reaction the maximum rate occurs where
$$C_A = C_R$$
. Thus operate at $C_A = 5$, if possible. Here
 $-T_A = 0.001C_AC_R = 0.001 \times 5 \times 5 = 0.025$
So for mixed flow
 $T = \frac{10-5}{0.025} = \frac{5}{0.025} = 200s = \frac{V}{U} = \frac{V}{1.5}$
Thus $V = 300$ lit, or 3 mfr side by side. Thus we should hook the
A reactors as shown
 $U = 1.5$ lit/s
 $C_{A0} = 10 \text{ mol/lit}$
For the fourth reactor $T = \frac{V/U}{U} = \frac{100/15}{60.75} = \frac{5-C_{A2}}{0.001C_{A2}(10-C_{A2})}$, or $C_{A2} = 3.486 \frac{\text{mol}}{14}$

6.13. 100 liters/hr of radioactive fluid having a half-life of 20 hr is to be treated by passing it through two ideal stirred tanks in series, $V = 40\,000$ liters each. In passing through this system, how much will the activity decay?

6.13 From 1/2 life data for radioactive decay (first order kinetics) we have

$$-\frac{dC}{dt} = kC \quad \text{or} \quad \ln \frac{C_0}{C} = kt \quad \text{or} \quad \ln 2 = k(20hrs) \quad \text{or} \quad k = \frac{\ln 2}{20hr}$$
and for 2 equal sized tanks in series Eq 6.6a gives

$$\frac{C_{out}}{C_0} = \frac{1}{(1+kT_1)^2} = \frac{1}{(1+\frac{\ln 2}{20}(400))^2} = \frac{1}{(1+20\ln 2)^2} = 0.00453$$
* only 0.453% of the activity remains,
99.5% of the activity has disappeared

6.15. The kinetics of the aqueous-phase decomposition of A is investigated in two mixed flow reactors in series, the second having twice the volume of the first reactor. At steady state with a feed concentration of 1 mol A/liter and mean residence time of 96 sec in the first reactor, the concentration in the first reactor is 0.5 mol A/liter and in the second is 0.25 mol A/liter. Find the kinetic equation for the decomposition.

$$-r_{A} = \left(\frac{1}{48} \frac{lit}{molisec}\right) C_{A}^{2} = \left(1.25 \frac{lit}{mol\cdot min}\right) C_{A}^{2} - \frac{1}{100}$$

6.17. The elementary irreversible aqueous-phase reaction $A + B \rightarrow R + S$ is carried out isothermally as follows. Equal volumetric flow rates of two liquid streams are introduced into a 4-liter mixing tank. One stream contains 0.020 mol A/liter, the other 1.400 mol B/liter. The mixed stream is then passed through a 16-liter plug flow reactor. We find that some R is formed in the mixing tank, its concentration being 0.002 mol/liter. Assuming that the mixing tank acts as a mixed flow reactor, find the concentration of R at the exit of the plug flow reactor as well as the fraction of initial A that has been converted in the system.

6.19. We wish to explore various reactor setups for the transformation of A into R. The feed contains 99% A, 1% R; the desired product is to consist of 10% A, 90% R. The transformation takes place by means of the elementary reaction

$$A + R \rightarrow R + R$$

with rate constant k = 1 liter/mol \cdot min. The concentration of active materials is $C_{A0} + C_{R0} = C_A + C_R = C_0 = 1$ mol/liter

throughout.

What reactor holding time will yield a product in which $C_R = 0.9 \text{ mol/}$ liter (a) in a plug flow reactor, (b) in a mixed flow reactor, and (c) in a minimum-size setup without recycle?

6.19 Let us solve by using the graphical procedure, and lets use concentrations, not conversions. First prepare the K-rA US CA corves from the data of the table, below

C _A	CR	-rA = KCACR	- <u>CA</u>
0.99	0.01	0.0099	101.01
0.95	0,05	0.0475	21.05
0,90	0.1	0.09	11.11
0.70	0.3	0.21	4.76
0.50	0.5	0.25	4.00
0.30	0.7	0.21	4.76
0.10	0,9	0.09	11.11

6.21. For an irreversible first-order liquid-phase reaction ($C_{A0} = 10$ mol/liter) conversion is 90% in a plug flow reactor. If two-thirds of the stream leaving the reactor is recycled to the reactor entrance, and if the throughput to the whole reactor-recycle system is kept unchanged, what does this do to the concentration of reactant leaving the system?

6.21 Originally we had plug flow, istorder,
$$X_{A}=0.9$$

$$\frac{C_{A}}{C_{AO}} = e^{-kT}$$

$$C_{AO}=10 - C_{AI}$$
or $loT = ln \frac{C_{AO}}{C_{A}} = ln 10 = 2.3 - (i)$

With recycle

$$k\tau = (R+1) \ln \left[\frac{C_{ho} + RC_{AF}}{(R+1)C_{AF}} \right] = (2+1) \ln \left[\frac{10+2C_{AF}}{(2+1)C_{AF}} \right] - --(ii)$$

Combining is a first gives

$$3 = (2+1) \ln \left[\frac{10+2C_{AF}}{(2+1)G_{F}}\right]$$

$$U = 1 - 3$$

$$U = 1 - 3$$

$$R = 2$$

$$R = 2$$

Solving for Caf gives $C_{Af} = 2.24$, or $X_{Af} = 0.776$ -