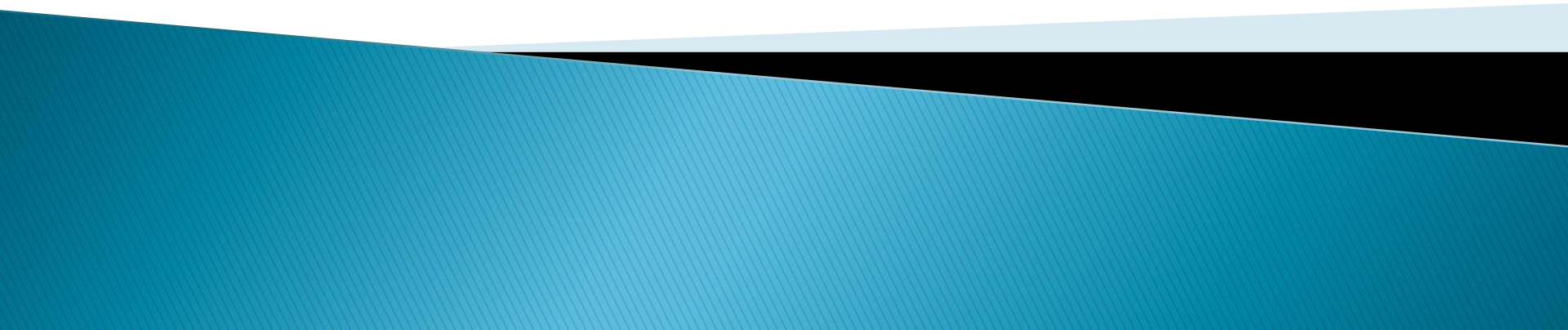


# Design for Parallel Reactions

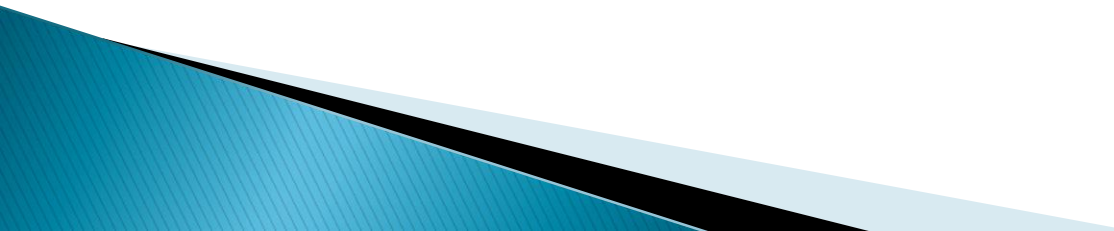
## Chapter 7



# Introduction to Multiple Reactions

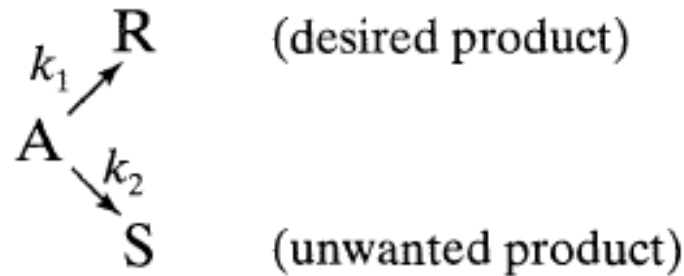
- ▶ We extend the discussion to multiple reactions and show that for these, both the size requirement and the distribution of reaction products are affected by the pattern of flow within the vessel.
- ▶ many multiple reactions can be considered to be combinations of two primary types:  
*parallel reactions* and *series reactions*
- ▶ we treat parallel reactions. In the next chapter we treat series reactions as well as all sorts of series-parallel combinations

- ▶ First, it more convenient to deal with concentrations rather than conversions
- ▶ Second, in examining product distribution the procedure is to eliminate the time variable by dividing one rate equation by another.
- ▶ Equations relating the rates of change of certain components with respect to other components of the systems
- ▶ Thus, we use two distinct analyses,
  - One for determination of reactor size and
  - Other for the study of product distribution.
- ▶ The two requirements,
  - ✓ small reactor size and
  - ✓ maximization of desired product,
- ▶ may run counter to each other.

- ▶ In such a situation an economic analysis will yield the best compromise.
  - ▶ this chapter concerns primarily optimization with respect to product distribution,
  - ▶ we ignore expansion effects in this chapter; thus, we take  $\varepsilon = 0$
  - ▶ This means that we may use the terms mean residence time, reactor holding time, space time, and reciprocal space velocity interchangeably
- 

# Qualitative Discussion About Product Distribution

- ▶ Consider the decomposition of A by either one of two paths:



## Corresponding rate equations

$$r_R = \frac{dC_R}{dt} = k_1 C_A^{a_1}$$

$$r_S = \frac{dC_S}{dt} = k_2 C_A^{a_2}$$

- ▶ Measure of the relative rates of formation of R and S. Thus

$$\frac{r_R}{r_S} = \frac{dC_R}{dC_S} = \frac{k_2}{k_1} C_A^{a_1 - a_2}$$

This ratio to be as large as possible

- ▶ Now  $C_A$  is the only factor in this equation which we can adjust and control
- ▶  $k_1$ ,  $k_2$ ,  $a_1$ , and  $a_2$  are all constant for a specific system at a given temperature
- ▶ we can keep  $C_A$  low throughout the reactor by any of the following means: by using
  - ✓ mixed flow reactor,
  - ✓ maintaining high conversions,
  - ✓ increasing inerts in the feed,
  - ✓ decreasing the pressure in gas-phase systems.

- ▶ we can keep  $C_A$  high by using
  - ✓ batch or plug flow reactor,
  - ✓ maintaining low conversions,
  - ✓ removing inerts from the feed,
  - ✓ increasing the pressure in gas phase systems.
- ▶ let us see whether the concentration of **A** should be kept high or low.
  - If  $a_1 > a_2$  or the desired reaction is of higher order than the unwanted reaction,
- ▶ shows that a high reactant concentration is desirable since it increases the R/S ratio.
- ▶ **As** a result, a **batch or plug flow** reactor would favor formation of product R and would require a minimum reactor size.

- ▶ If  $a_1 < a_2$ , or the desired reaction is of lower order than the unwanted reaction,
- ▶ we need a low reactant concentration to favor formation of R. But this would also require large **mixed flow reactor**.
- ▶ If  $a_1 = a_2$ , or the two reactions are of the same order.

$$\frac{r_R}{r_S} = \frac{dC_R}{dC_S} = \frac{k_1}{k_2} = \text{constant}$$

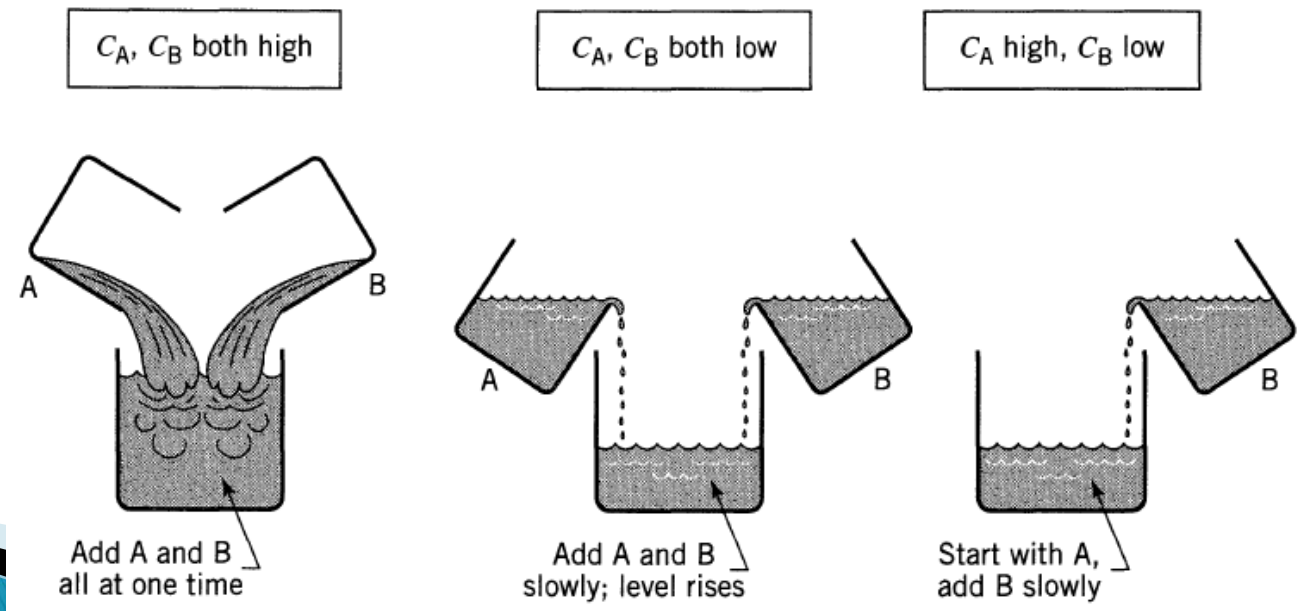
- ▶ Hence, product distribution is fixed by  $k_1/k_2$ , alone and is unaffected by type of reactor used.
- ▶ We also may control product distribution by varying  $k_2/k_1$ . This can be done in two ways:
  - By **changing the temperature** level of operation. If the activation energies of the two reactions are different,  $k_1/k_2$  can be made to vary.
  - By using a **catalyst**.

One of the most important features of a catalyst is its selectivity in depressing or accelerating specific reactions.

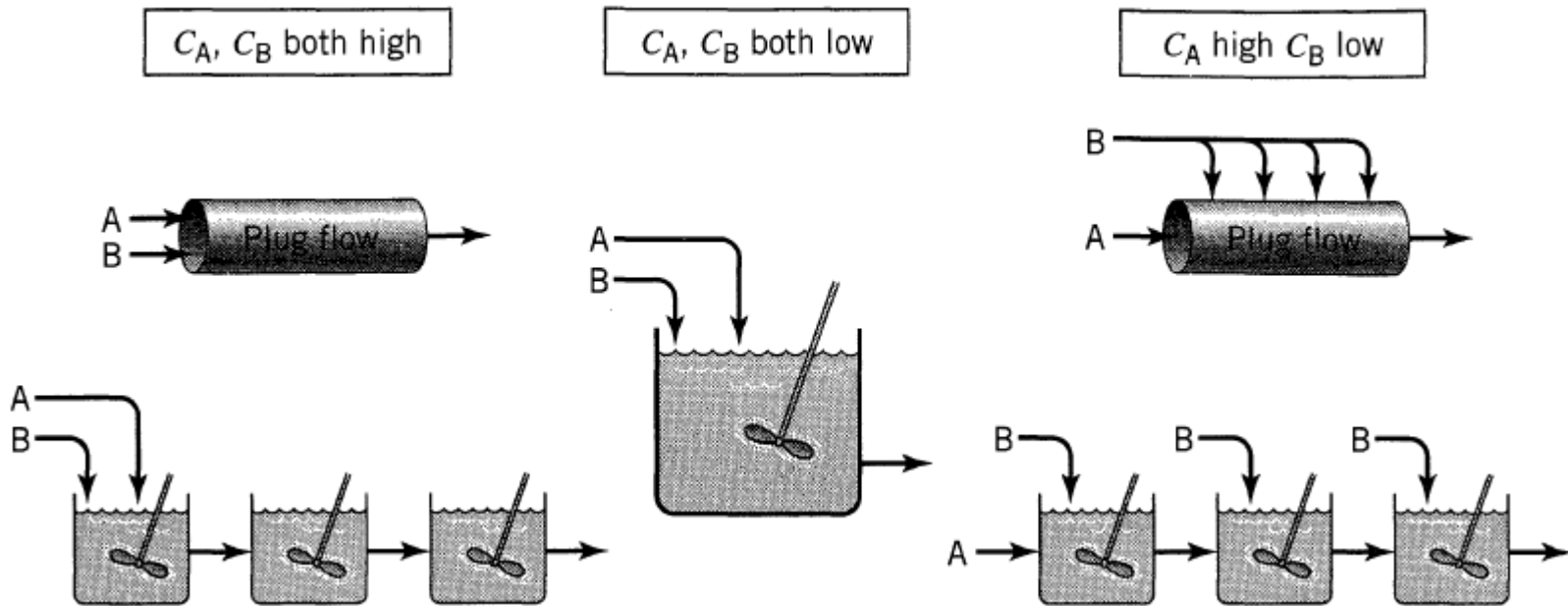


- ▶ When you have two or more reactants, combinations of high and low reactant concentrations can be obtained by controlling the concentration of feed materials.
- ▶ methods of contacting two reacting fluids in continuous and non-continuous operations that keep the concentrations of these components both high, both low, or one high and the other low

## Non-continuous operations

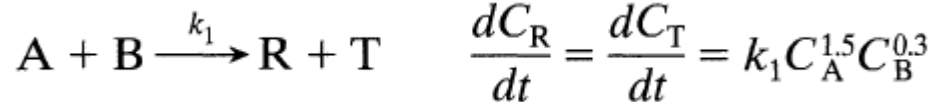


# continuous flow operations

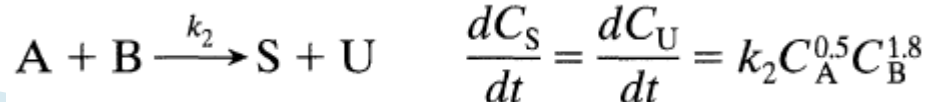


## CONTACTING PATTERNS FOR REACTIONS IN PRALLEL

The desired liquid-phase reaction



Unwanted side reaction



$$\frac{r_R}{r_S} = \frac{k_1}{k_2} C_A C_B^{-1.5}$$

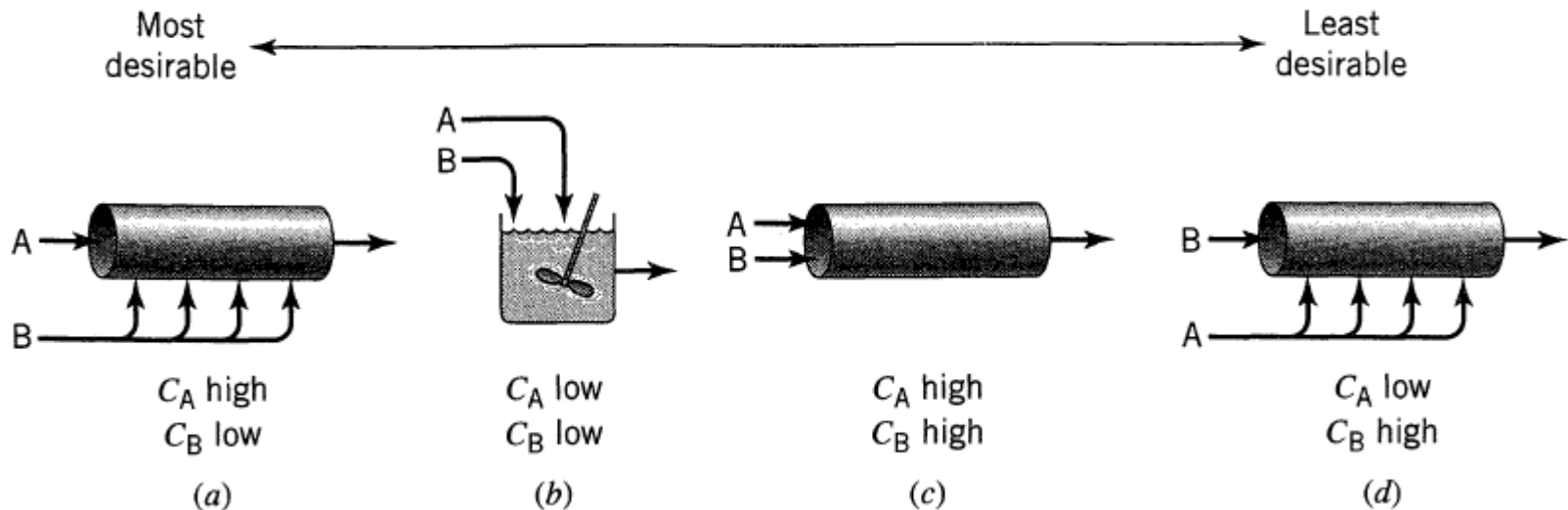
According to the rule for reactions in parallel,  
we want to keep

$C_A$  high,  $C_B$  low,

Since the concentration dependency of B is more pronounced than of A,

It is more important to have low  $C_B$  than high  $C_A$

The contacting schemes are therefore



# Quantitative Treatment of Product Distribution and of Reactor Size

- ▶ If rate equations are known for the individual reactions,
- ▶ we can quantitatively determine product distribution and reactor-size requirements.
- ▶ For convenience in evaluating product distribution, introduce two terms  $\varphi$  and  $\Phi$ .
- ▶ let  $\varphi$  be the fraction of A disappearing at any instant which is transformed into desired product R.
- ▶ We call this the *instantaneous fractional yield of R*.

at any  $C_A$

$$\varphi = \left( \frac{\text{moles R formed}}{\text{moles A reacted}} \right) = \frac{dC_R}{-dC_A}$$

- ▶ For any particular set of reactions and rate equations  $\varphi$  is a function of  $C_A$ ,
- ▶ Since  $C_A$  in general varies through the reactor,  $\varphi$  will also change with position in the reactor.

- ▶ Let us define  $\Phi$  as the fraction of all the reacted A that has been converted into R, and let us call this the *overall fractional yield of R*
- ▶ The overall fractional yield is then the mean of the instantaneous fractional yields at all points within the reactor

$$\Phi = \left( \frac{\text{all R formed}}{\text{all A reacted}} \right) = \frac{C_{Rf}}{C_{A0} - C_{Af}} = \frac{C_{Rf}}{(-\Delta C_A)} = \bar{\varphi}_{\text{in reactor}}$$

- ▶ Proper averaging for  $\varphi$  depends on the type of flow within the reactor. Thus for plug *flow*, where  $C_A$  changes progressively through the reactor

$$\text{For PFR: } \Phi_p = \frac{-1}{C_{A0} - C_{Af}} \int_{C_{A0}}^{C_{Af}} \varphi dC_A = \frac{1}{\Delta C_A} \int_{C_{A0}}^{C_{Af}} \varphi dC_A$$

- ▶ mixed *flow*, the composition is  $C_{\cdot}$ , everywhere, so  $\varphi$  is likewise constant throughout the reactor

$$\text{For MFR: } \Phi_m = \varphi_{\text{evaluated at } C_{Af}}$$

- ▶ The over-all fractional yields from mixed and plug flow reactors processing A from  $C_A$  to  $C_{Af}$  are related by

$$\Phi_m = \left( \frac{d\Phi_p}{dC_A} \right)_{\text{at } C_{Af}} \quad \text{and} \quad \Phi_p = \frac{1}{\Delta C_A} \int_{C_{A0}}^{C_{Af}} \Phi_m dC_A$$

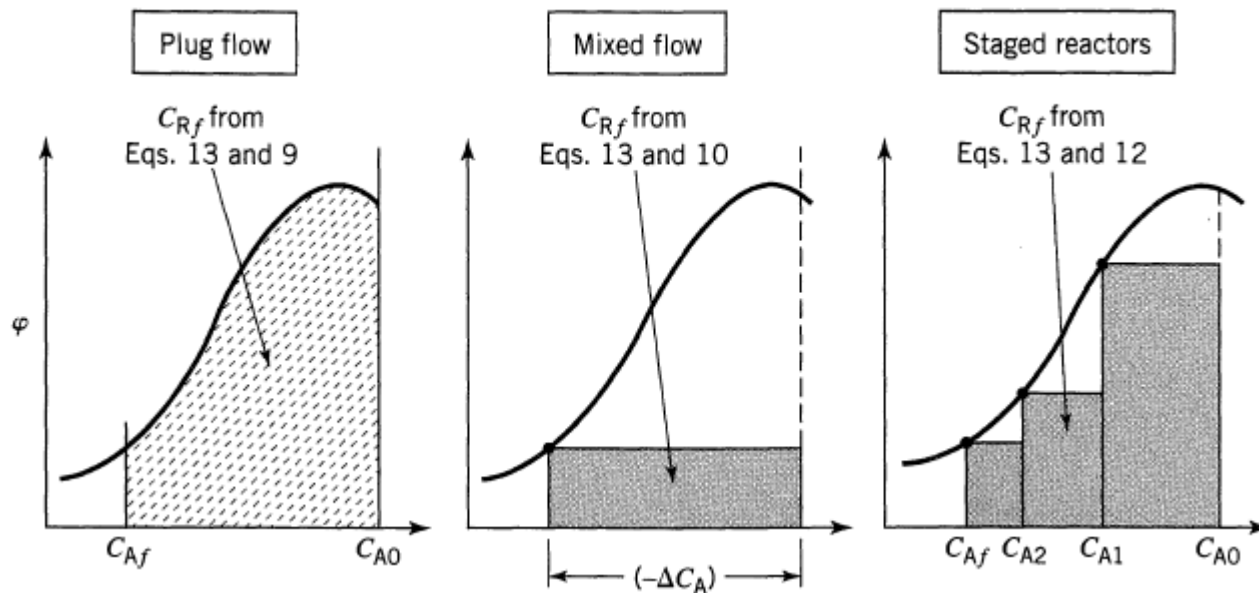
- ▶ For a series of 1, 2, . . . , N mixed flow reactors in which the concentration of A is  $C_{A1}$ ,  $C_{A2}$  . . . ,  $C_{AN}$  the overall fractional yield is obtained by summing the fractional yields in each of the N vessels and weighting these values by the amount of reaction occurring in each vessel

$$\varphi_1(C_{A0} - C_{A1}) + \dots + \varphi_N(C_{A,N-1} - C_{AN}) = \Phi_{N \text{ mixed}} (C_{A0} - C_{AN})$$

$$\Phi_{N \text{ mixed}} = \frac{\varphi_1(C_{A0} - C_{A1}) + \varphi_2(C_{A1} - C_{A2}) + \dots + \varphi_N(C_{A,N-1} - C_{AN})}{C_{A0} - C_{AN}}$$

For any reactor type the exit concentration of R is obtained directly

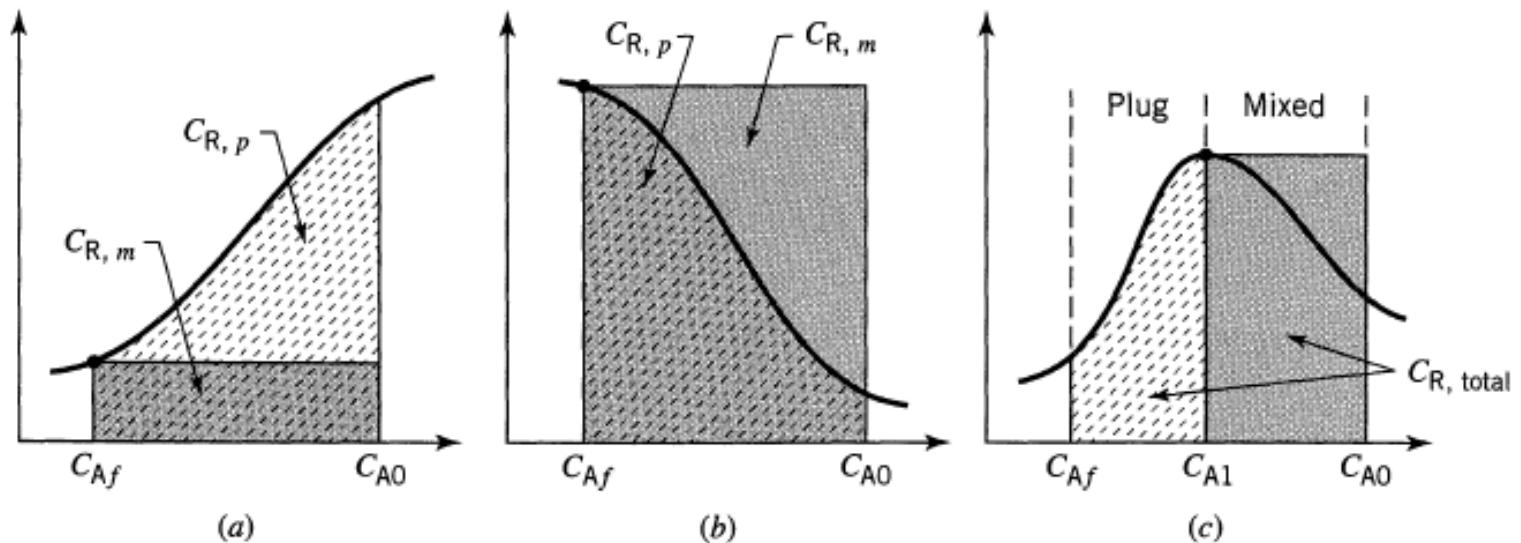
$$C_{Rf} = \Phi(C_{A0} - C_{Af})$$



**Shaded and dashed area gives total R formed.**



- Now the shape of the  $\phi$  versus  $C_A$  curve determines which type of flow gives the best product distribution



The contacting pattern with the largest area produces most R

(a) plug flow is best,

(b) mixed flow is best,

(c) mixed flow up to  $C_{A1}$  followed by plug flow is best

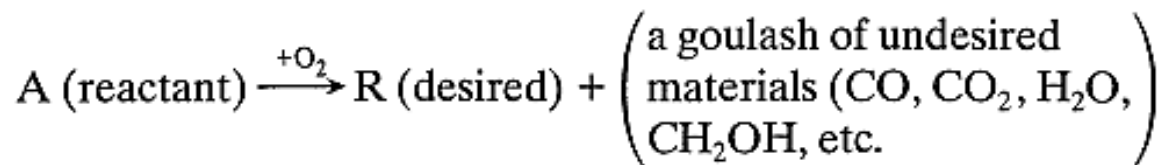


# Selectivity

- ▶ selectivity, is often used in place of fractional yield. It is usually defined as follows

$$\text{selectivity} = \left( \frac{\text{moles of desired product formed}}{\text{moles of undesired material formed}} \right)$$

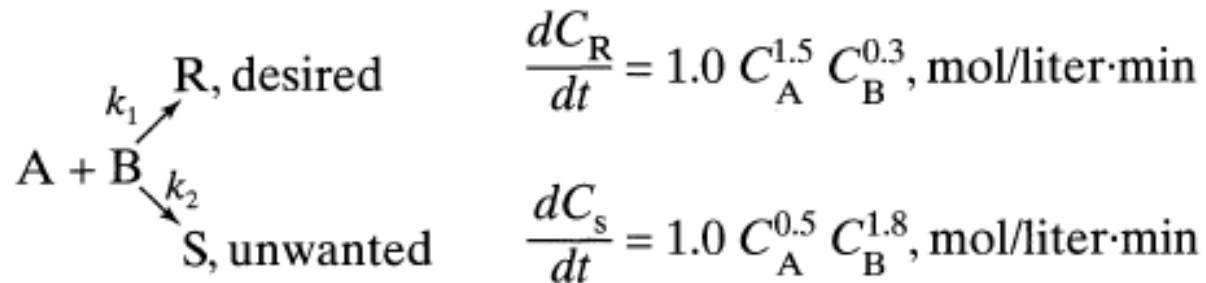
- ▶ This definition may lead to difficulties. For example, if the reaction is the partial oxidation of a hydrocarbon



Here the selectivity is hard to evaluate, and not very useful. Thus, we stay away from selectivity and use the clearly defined and useful fractional yield,  $\varphi(\text{R/A})$ .

# PRODUCT DISTRIBUTION FOR PARALLEL REACTIONS

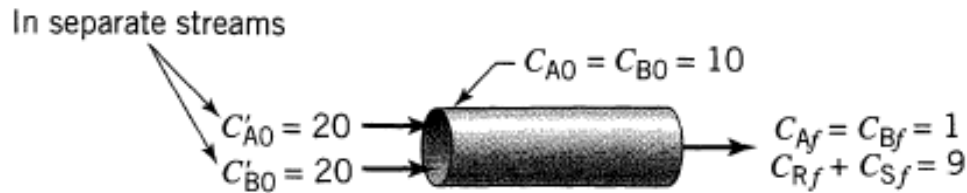
Consider the aqueous reactions



For 90% conversion of A find the concentration of R in the product stream. Equal volumetric flow rates of the A and of B streams are fed to the reactor, and each stream has a concentration of 20 mol/liter of reactant.

The flow in the reactor follows.

- (a) Plug flow
- (b) Mixed flow
- (c) The best of the four plug-mixed contacting schemes



be careful to get the concentrations right when you mix streams  
The instantaneous fractional yield of the desired compound

$$\varphi \left( \frac{R}{A} \right) = \frac{dC_R}{dC_R + dC_S} = \frac{k_1 C_A^{1.5} C_B^{0.3}}{k_1 C_A^{1.5} C_B^{0.3} + k_2 C_A^{0.5} C_B^{1.8}} = \frac{C_A}{C_A + C_B^{1.5}}$$

### (a) Plug Flow

That the starting concentration of each reactant in the combined feed is  $C_{A0} = C_{B0} = 10$  mol/liter and that  $C_A = C_B$  everywhere,

$$\Phi_p = \frac{-1}{C_{A0} - C_{Af}} \int \varphi dC_A = \frac{-1}{10 - 1} \int_{10}^1 \frac{C_A dC_A}{C_A + C_A^{1.5}} = \frac{1}{9} \int_1^{10} \frac{dC_A}{1 + C_A^{0.5}}$$

Let  $C_A^{0.5} = x$ , then  $C_A = x^2$  and  $dC_A = 2x dx$ . Replacing  $C_A$  by  $x$  in the above expression gives

$$\begin{aligned} \Phi_p &= \frac{1}{9} \int_1^{\sqrt{10}} \frac{2x dx}{1 + x} = \frac{2}{9} \left[ \int_1^{\sqrt{10}} dx - \int_1^{\sqrt{10}} \frac{dx}{1 + x} \right] \\ &= 0.32 \end{aligned}$$

$$C_{Rf} = 9(0.32) = \underline{\underline{2.86}}$$

$$C_{Sf} = 9(1 - 0.32) = \underline{\underline{6.14}}$$

**(b) Mixed Flow**

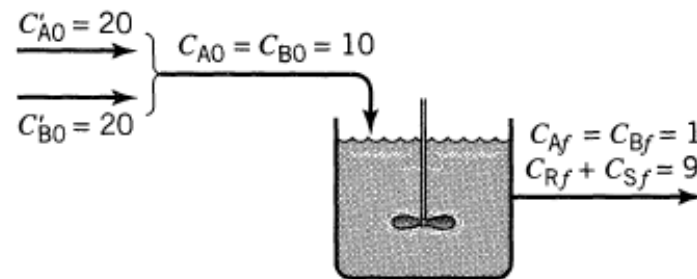
Referring to Fig. E7.2b, we have from Eq. 10, for  $C_A = C_B$

For MFR:  $\Phi_m = \varphi_{\text{evaluated at } C_{Af}}$   $\Phi_m \left( \frac{R}{A} \right) = \varphi_{\text{at exit}} = \frac{1}{1 + C_A^{0.5}} = 0.5$

Therefore Eq. 13 gives

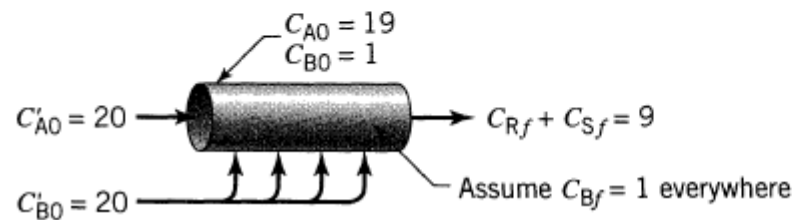
$$C_{Rf} = 9(0.5) = \underline{\underline{4.5 \text{ mol/liter}}}$$

$$C_{Sf} = 9(1 - 0.5) = \underline{\underline{4.5 \text{ mol/liter}}}$$



**(c) Plug Flow A—Mixed Flow B**

Assuming that B is introduced into the reactor in such a way that  $C_B = 1$  mol/liter throughout, we find concentrations as shown in Fig. E7.2c. Then accounting



for the changing  $C_A$  in the reactor, we find

$$\begin{aligned}\Phi\left(\frac{R}{A}\right) &= \frac{-1}{C_{A0} - C_{Af}} \int_{C_{A0}}^{C_{Af}} \varphi dC_A = \frac{-1}{19 - 1} \int_{19}^1 \frac{C_A dC_A}{C_A + (1)^{1.5}} \\ &= \frac{1}{18} \left[ \int_1^{19} dC_A - \int_1^{19} \frac{dC_A}{C_A + 1} \right] = \frac{1}{18} \left[ (19 - 1) - \ln \frac{20}{2} \right] = 0.87\end{aligned}$$

$$C_{Rf} = 9(0.87) = \underline{\underline{7.85 \text{ mol/liter}}}$$

$$C_{Sf} = 9(1 - 0.87) = \underline{\underline{1.15 \text{ mol/liter}}}$$

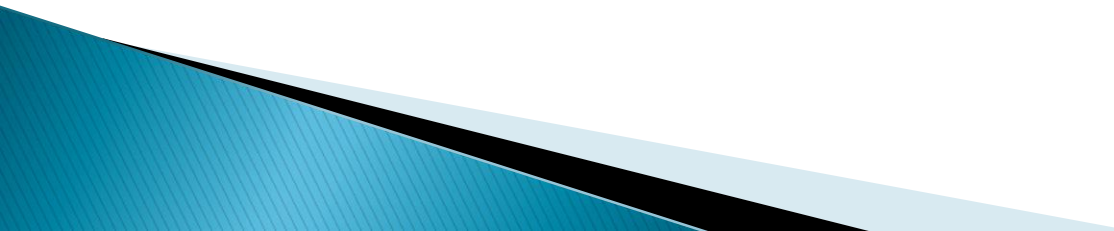
To summarize

$$\text{For plug flow: } \Phi\left(\frac{R}{A}\right) = 0.32 \quad \text{and} \quad C_{Rf} = 2.86 \text{ mol/liter}$$

$$\text{For mixed flow: } \Phi\left(\frac{R}{A}\right) = 0.50 \quad \text{and} \quad C_{Rf} = 4.5 \text{ mol/liter}$$

$$\text{For the optimum: } \Phi\left(\frac{R}{A}\right) = 0.87 \quad \text{and} \quad C_{Rf} = 7.85 \text{ mol/liter}$$

# The Side Entry Reactor

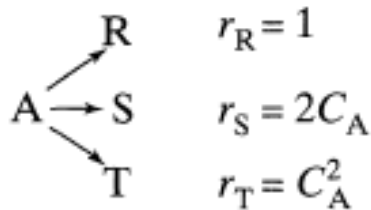
- ▶ To evaluate how best to distribute the side entry feed and how to calculate the corresponding conversion equation is a rather complex problem.
  - ▶ somewhat like a shell-and-tube heat exchanger which used porous walled tubes.
- 

# GOOD OPERATING CONDITIONS FOR PARALLEL REACTIONS

Often a desired reaction is accompanied by a variety of undesired side reactions, some of higher order, some of lower order.

To see which type of single reactor gives the best product distribution, consider the simplest typical case, the parallel decompositions of A,

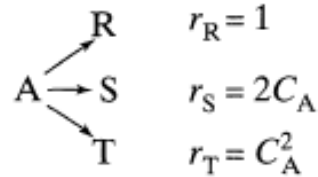
$$C_{A0} = 2,$$



Find the maximum expected  $C_S$  for isothermal operations

- (a) in a mixed flow reactor
- (b) in a plug flow reactor
- (c) in a reactor of your choice if unreacted A can be separated from the product stream and returned to the feed at  $C_{A0} = 2$ .

$$C_{A0} = 2,$$



Since S is the desired product, let us write fractional yields in terms of S. Thus

$$\varphi(S/A) = \frac{dC_S}{dC_R + dC_S + dC_T} = \frac{2C_A}{1 + 2C_A + C_A^2} = \frac{2C_A}{(1 + C_A)^2}$$

Plotting this function we find the curve of Fig. E7.3 whose maximum occurs where

$$\frac{d\varphi}{dC_A} = \frac{d}{dC_A} \left[ \frac{2C_A}{(1 + C_A)^2} \right] = 0$$

Solving we find

$$\varphi = 0.5 \quad \text{at} \quad C_A = 1.0$$

**(a) Mixed Reactor.** Most S is formed when the rectangle under the  $\varphi$  versus  $C_A$  curve has the largest area. The required conditions can be found either by graphical maximization of rectangles or analytically. Since simple explicit expressions are available in this problem, let us use the latter approach. Then from Eqs. 10 and 13 we find for the area of the rectangle

$$C_{Sf} = \varphi(S/A) \cdot (-\Delta C_A) = \frac{2C_A}{(1 + C_A)^2} (C_{A0} - C_A)$$

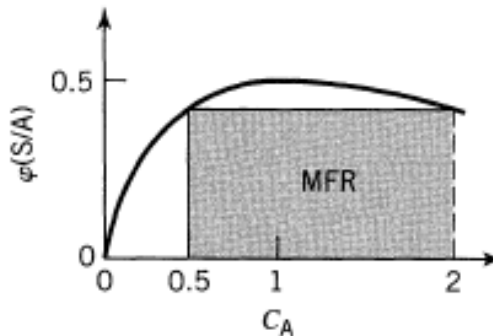


Differentiating and setting to zero to find the conditions at which most S is formed

$$\frac{dC_{Sf}}{dC_A} = \frac{d}{dC_A} \left[ \frac{2C_A}{(1 + C_A)^2} (2 - C_A) \right] = 0$$

Evaluating this quantity gives the optimum operating conditions of a mixed reactor as

$$\underline{C_{Sf} = \frac{2}{3}} \quad \text{at} \quad C_{Af} = \frac{1}{2}$$



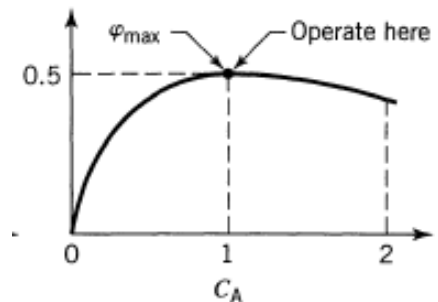
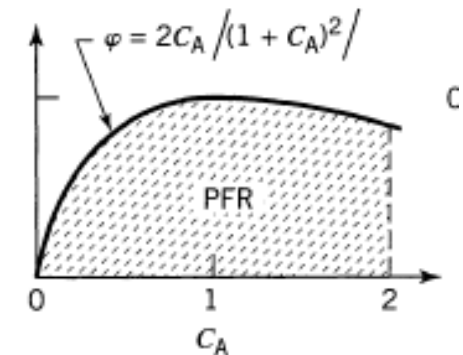
**(b) Plug Flow Reactor.** The production of S is maximum when the area under the  $\phi$  versus  $C_A$  curve is maximum. This occurs at 100% conversion of A,

$$C_{Sf} = - \int_{C_{A0}}^{C_{Af}} \varphi(S/A) dC_A = \int_0^2 \frac{2C_A}{(1 + C_A)^2} dC_A$$

Evaluating this integral gives, for the plug flow optimum,

$$\underline{\underline{C_{Sf} = 0.867}} \quad \text{at} \quad C_{Af} = 0$$

**(c) Any Reactor with Separation and Recycle of Unused Reactant.** Since no reactant leaves the system unconverted, what is important is to operate at conditions of highest fractional yield. This is at  $C_A = 1$ , where  $\varphi(S/A) = 0.5$ , as shown in Fig. E7.3c. Thus, we should use a mixed flow reactor operating at  $C_A = 1$ . We would then have 50% of reactant A forming product S.



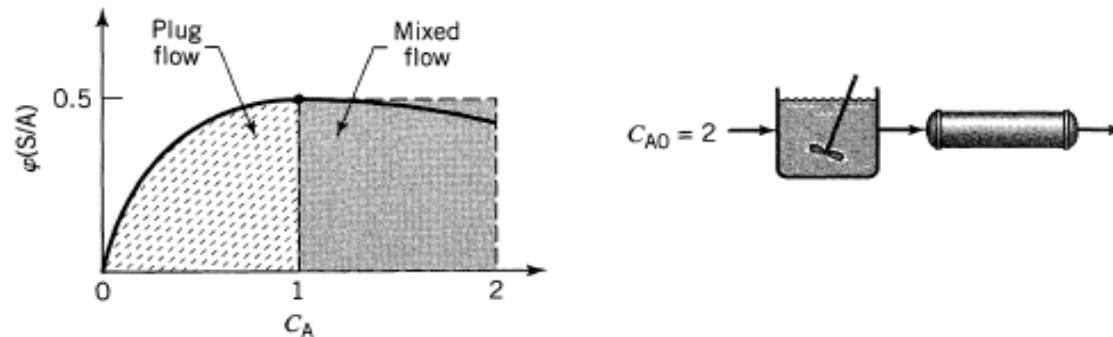
**Comment.** Summarizing, we find

$$\begin{aligned} \left( \frac{\text{moles S formed}}{\text{moles A fed}} \right) &= 0.33 \text{ for MFR} \\ &= 0.43 \text{ for a PFR} \\ &= 0.50 \text{ for an MFR with separation and recycle} \end{aligned}$$

# Best Operating Conditions for Parallel

For the reaction of Example 7.3 determine the arrangement of reactors which would produce most S in a flow system where recycle and reconcentration of unreacted feed is not possible. Find  $C_{S,\text{total}}$  for this arrangement of reactors.

From Fig. E7.4 we see that mixed flow followed by plug flow would be best.



Thus, for mixed flow, from Example 7.3

$$C_A = 1, \varphi = 0.5, \quad \text{thus} \quad C_S = \varphi(\Delta C_A) = 0.5(2 - 1) = 0.5 \text{ mol/liter}$$

For plug flow, from Example 7.3

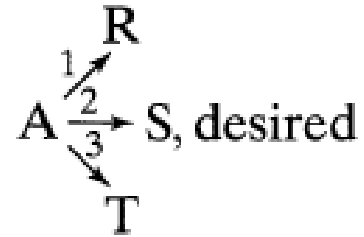
$$C_S = - \int_1^0 \varphi dC_A = \int_0^1 \frac{2C_A}{(1 + C_A)^2} dC_A = 0.386 \text{ mol/liter}$$

Therefore, the total amount of  $C_S$  formed is

$$C_{S,\text{total}} = 0.5 + 0.386 = \underline{\underline{0.886 \text{ mol/liter}}}$$

This is only slightly better than for plug flow alone, calculated in Example 7.3.

7.1. For a given feed stream having  $C_{A0}$  should we use a PFR or a MFR and should we use a high or low or some intermediate conversion level for the exit stream if we wish to maximize  $\phi(S/A)$  The reaction system is



where  $n_1$ ,  $n_2$ , and  $n_3$  are the reaction orders of reactions 1, 2, and 3

**(a)**  $n_1 = 1, n_2 = 2, n_3 = 3$

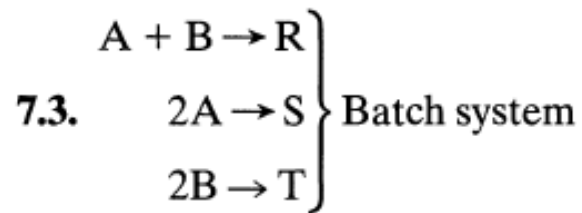
**(b)**  $n_1 = 2, n_2 = 3, n_3 = 1$

**(c)**  $n_1 = 3, n_2 = 1, n_3 = 2$

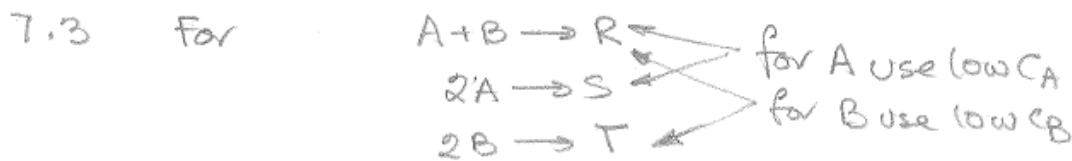
7.1 a) Use a MFR with some particular concentration of A

b) Use a PFR, with low  $X_A$

c) Use a MFR, with high  $X_A$



Using separate feeds of A and B sketch the contacting pattern and reactor conditions which would best promote the formation of product R for the following systems of elementary reactions.

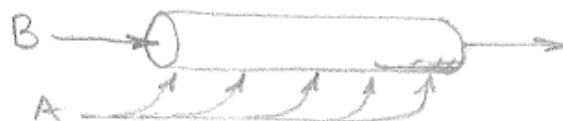
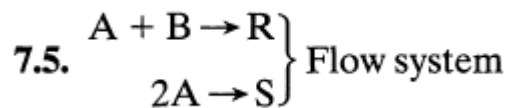


Thus

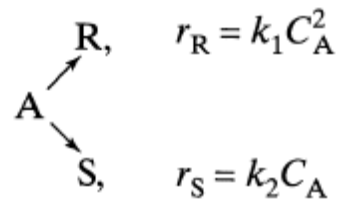


drip A and B in slowly  
keep  $X_A$  high  
keep  $X_B$  high

Don't have an excess of either A or B

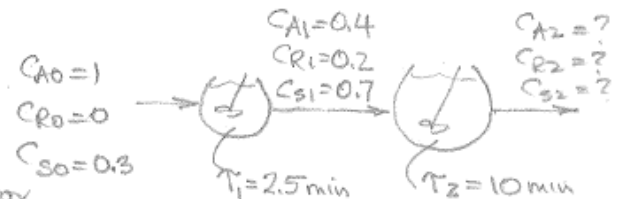
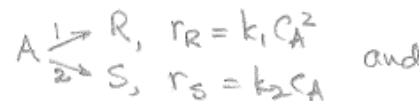


7.7. Substance A in the liquid phase produces R and S by the following reactions:



The feed ( $C_{A0} = 1.0$ ,  $C_{R0} = 0$ ,  $C_{S0} = 0.3$ ) enters two mixed flow reactors in series ( $\tau_1 = 2.5$  min,  $\tau_2 = 10$  min). Knowing the composition in the first reactor ( $C_{A1} = 0.4$ ,  $C_{R1} = 0.2$ ,  $C_{S1} = 0.7$ ), find the composition leaving the second reactor.

7.7 Given



For mixed flow in the first reactor

$$\tau_1 = \frac{C_{R1} - C_{R0}}{k_1 C_A^2} \quad \therefore k_1 = \frac{0.2 - 0}{2.5 (0.4)^2} = 0.5$$

Also

$$\tau_1 = \frac{C_{S1} - C_{S0}}{k_2 C_A} \quad \therefore k_2 = \frac{0.7 - 0.3}{2.5 (0.4)} = 0.4$$

For the second reactor

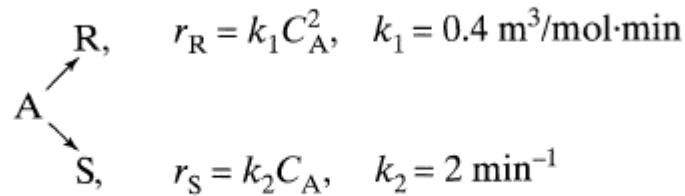
$$\tau_2 = \frac{C_{A1} - C_{A2}}{k_1 C_A^2 + k_2 C_A} = \frac{0.4 - C_{A2}}{0.5 C_{A2}^2 + 0.4 C_{A2}} = 10 \quad \therefore C_{A2} = 0.0745 \leftarrow$$

Also

$$\tau_2 = \frac{C_{R2} - C_{R1}}{k_1 C_A^2} \quad \therefore C_{R2} = 0.2 + 10 (0.5) (0.0745)^2 = 0.2278 \leftarrow$$

$$\text{and } C_{S2} = 0.7 + 10 (0.4) (0.0745) = 0.998 \leftarrow$$

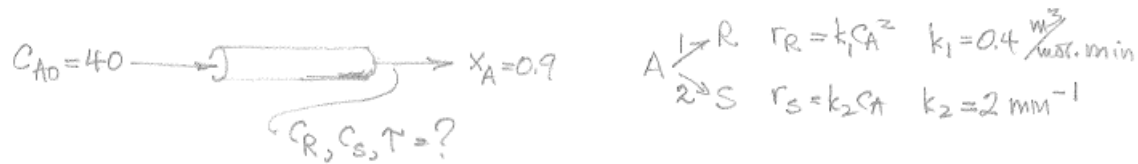
Liquid reactant A decomposes as follows:



A feed of aqueous A ( $C_{\text{A}0} = 40 \text{ mol/m}^3$ ) enters a reactor, decomposes, and a mixture of A, R, and S leaves.

**7.9.** Find  $C_{\text{R}}$ , and  $C_{\text{S}}$  and  $\tau$  for  $X_{\text{A}} = 0.9$  in a plug flow reactor.

7.9



First determine  $\phi(S/A)$ .

$$\phi(S/A) = \frac{r_{\text{S}}}{r_{\text{R}} + r_{\text{S}}} = \frac{2C_{\text{A}}}{0.4C_{\text{A}}^2 + 2C_{\text{A}}} = \frac{1}{1 + 0.2C_{\text{A}}}$$

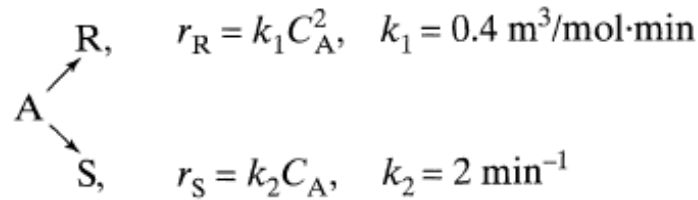
$$C_{\text{S}} = \int_4^{40} \phi(S/A) dC_{\text{A}} = \int_4^{40} \frac{dC_{\text{A}}}{1 + 0.2C_{\text{A}}} = \frac{1}{0.2} \ln(1 + 0.2C_{\text{A}}) \Big|_4^{40} = 5 \ln \frac{9}{1.8} = 8$$

$$\left. \begin{array}{l}
 \therefore C_{\text{A}} = 4 \\
 C_{\text{S}} = 8 \\
 C_{\text{R}} = 28
 \end{array} \right\} \longleftarrow$$

$$\tau = \int \frac{dC_{\text{A}}}{-r_{\text{A}}} = \int \frac{dC_{\text{A}}}{2C_{\text{A}} + 0.4C_{\text{A}}^2} = \frac{1}{0.4} \int \frac{dC_{\text{A}}}{5C_{\text{A}} + C_{\text{A}}^2} = 2.5 \left[ \frac{1}{5} \ln \frac{C_{\text{A}}}{C_{\text{A}} + 5} \right]_4^{40} = \frac{1}{2} \ln 2 = 0.347 \longleftarrow$$

7.11. Find the operating condition ( $X_A$ ,  $\tau$ , and  $C_R$ ) which maximizes  $C_R$  in a mixed flow reactor.

Liquid reactant A decomposes as follows:

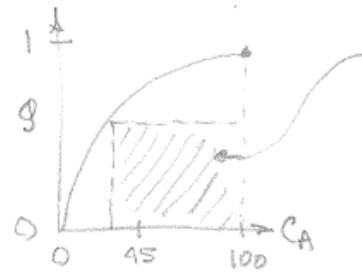


A feed of aqueous A ( $C_{A0} = 40 \text{ mol/m}^3$ ) enters a reactor, decomposes, and a mixture of A, R, and S leaves.

7.11 To maximize  $C_R$  in a MFR first look at the  $Q(R/A)$  vs  $C_A$  curve

$C_A$	$Q(R/A)$
100	100/105
45	45/50
20	20/25
5	5/10
0	0

... draw the ... curve



Solve by maximizing the area of the rectangle

$$\left[ \begin{aligned}
 Q(R/A) &= \frac{0.4C_A^2}{0.4C_A^2 + 2C_A} \\
 &= \frac{C_A}{C_A + 5}
 \end{aligned} \right]$$

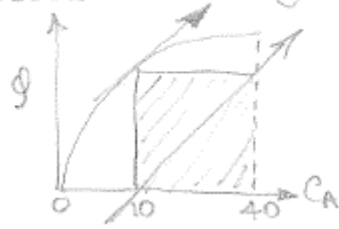
Method 1 Solve analytically

$$C_R = Q(-\Delta C_A) = \frac{C_A}{C_A + 5} (40 - C_A)$$

$$\frac{dC_R}{dC_A} = \frac{(40 - 2C_A)(C_A + 5) - (40C_A - C_A^2)}{(C_A + 5)^2} = 0 \quad \text{--- or } \left. \begin{array}{l} C_A = 10 \\ C_R = 20 \\ C_S = 10 \end{array} \right\} \longleftarrow$$



Method 2 Solve graphically by maximizing the shaded rectangle

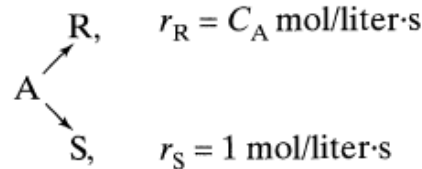


For  $\eta$ :

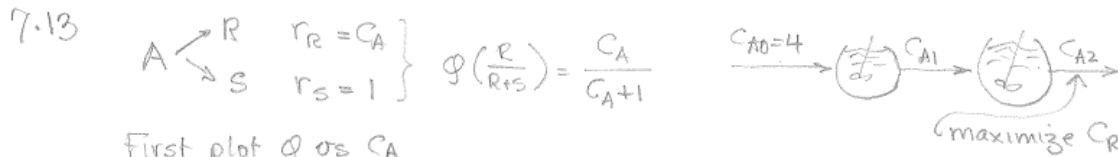
$$\eta = \frac{C_{A0} - C_{Af}}{-r_A} = \frac{C_{A0} - C_{Af}}{0.4C_{Af}^2 + 2C_{Af}} = \frac{40 - 10}{0.4(10)^2 + 2(10)}$$

$$= \frac{30}{60} = \frac{1}{2} \text{ min}$$

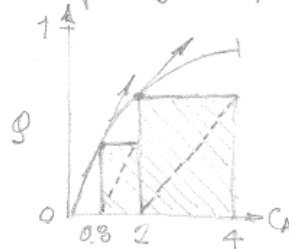
7.13. In a reactive environment, chemical A decomposes as follows



For a feed stream  $C_{A0} = 4$  mol/liter what size ratio of two mixed flow reactors will maximize the production rate of R? Also give the composition of A and R leaving these two reactors.



First plot  $\varphi$  vs  $C_A$



The shaded areas of the two rectangles gives  $C_R$ . We maximize this by trial and error. This gives  $C_{A1} = 2$  and  $C_{A2} = 0.8$

$$\left. \begin{array}{l}
 \therefore \tau_1 = \frac{V_1}{v} = \frac{C_{A0} - C_{A1}}{-r_{A1}} = \frac{C_{A0} - C_{A1}}{1 + C_{A1}} = \frac{4 - 2}{1 + 2} = \frac{2}{3} \\
 \text{and } \tau_2 = \frac{V_2}{v} = \frac{C_{A1} - C_{A2}}{-r_{A2}} = \frac{2 - 0.8}{1 + 0.8} = \frac{2}{3}
 \end{array} \right\} \therefore \frac{V_1}{V_2} = 1$$

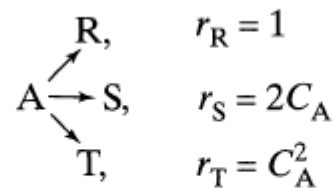
P.S. I'm not sure that this is the best solution.

and

$$\left. \begin{array}{l}
 C_{R1} = \varphi \cdot \Delta C_A = \frac{C_{A1}}{C_{A1}+1} (C_{A0} - C_{A1}) = \frac{2}{2+1} (4 - 2) = 1.33 \\
 C_{R2} = \frac{C_{A2}}{C_{A2}+1} (C_{A1} - C_{A2}) = \frac{0.8}{0.8+1} (\varphi - 0.8) = 0.533
 \end{array} \right\} \therefore C_{R \text{ max}} = 1.86 \frac{\text{mol}}{\text{lit}}$$

7.15 S is the desired product and  $C_{A0} = 4$ .

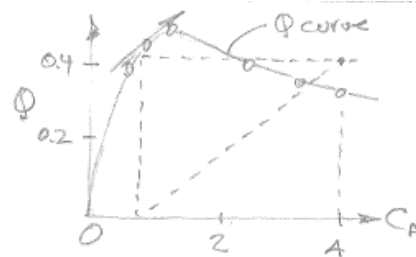
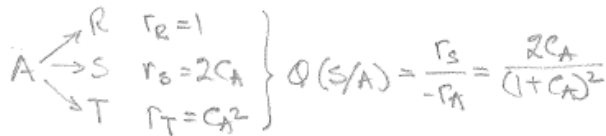
Consider the parallel decomposition of A of different orders



Determine the maximum concentration of desired product obtainable in

- (a) plug flow,  
 (b) mixed flow.

7.15



a) For plug flow go to  $C_{\text{A}f} = 0$  for maximum area

$$C_{\text{S}} = \int_0^4 \frac{2C_{\text{A}}}{(1+C_{\text{A}})^2} dC_{\text{A}} \approx (0.2984)4 = 1.59$$

graphical integration

b) For mixed flow let's solve analytically. Note we could also solve graphically.

$$C_{\text{S}} = \Phi(-\Delta C_{\text{A}}) = \frac{2C_{\text{A}}}{(1+C_{\text{A}})^2} (4-C_{\text{A}})$$

differentiating & setting to zero gives

$$\frac{dC_{\text{S}}}{dC_{\text{A}}} = \frac{[2(4-C_{\text{A}}) + 2C_{\text{A}}(-1)](1+C_{\text{A}})^2 - 2C_{\text{A}}(4-C_{\text{A}})2(1+C_{\text{A}})}{(1+C_{\text{A}})^4} = 0$$

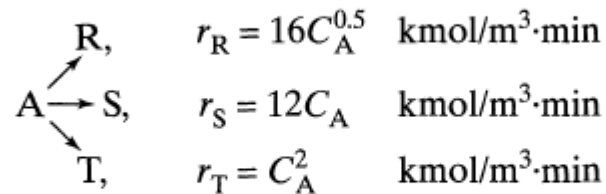
$$\therefore C_{\text{A}}(\text{at } C_{\text{Sopt}}) = \frac{2}{3}$$

$$\Phi(\text{at } C_{\text{A}} = \frac{2}{3}) = 2\left(\frac{2}{3}\right) / \left(1 + \frac{2}{3}\right)^2 = \frac{12}{25}$$

$$\therefore C_{\text{Smax}} = \frac{12}{25} \left(4 - \frac{2}{3}\right) = 1.6 \quad \leftarrow$$

7.17. Product R is the desired material.

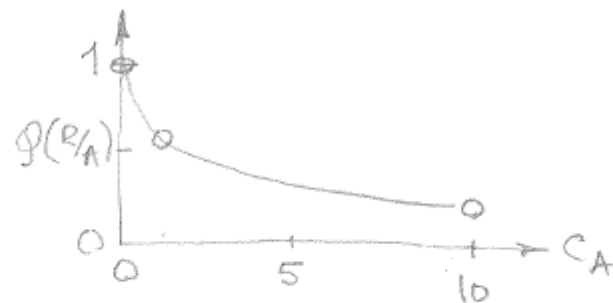
Under ultraviolet radiation, reactant A of  $C_{A0} = 10 \text{ kmol/m}^3$  in a process stream ( $v = 1 \text{ m}^3/\text{min}$ ) decomposes as follows.



We wish to design a reactor setup for a specific duty. Sketch the scheme selected, and calculate the fraction of feed transformed into desired product as well as the volume of reactor needed.

7.17 For reactions in parallel first evaluate & draw the  $q$  vs  $C_A$  curve

$C_A$	$q(R/A) = \frac{16C_A^{1/2}}{16C_A^{1/2} + 12C_A + C_A^2}$
10	0.185
1	0.55
0	1.0



The highest value for comes where  $C_A = 0$  and where  $q = 1$

∴ operate the mixed flow reactor at  $X_A \rightarrow 1$ . Here

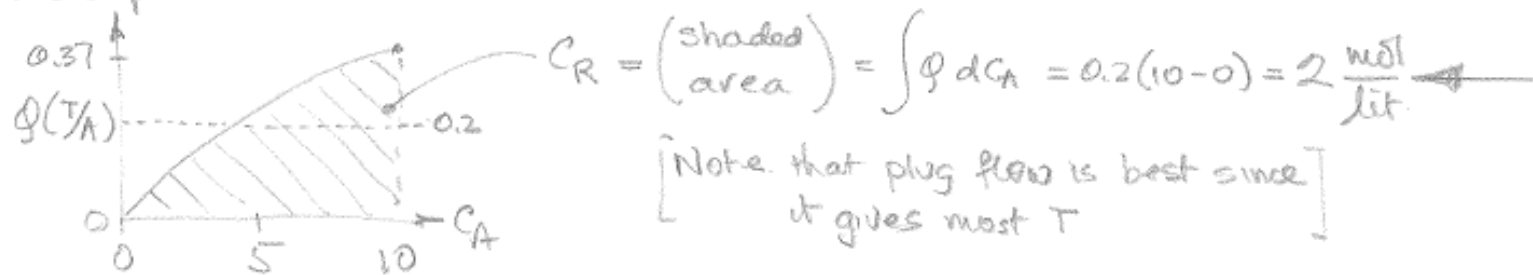


**7.19. Product T is the desired material.**

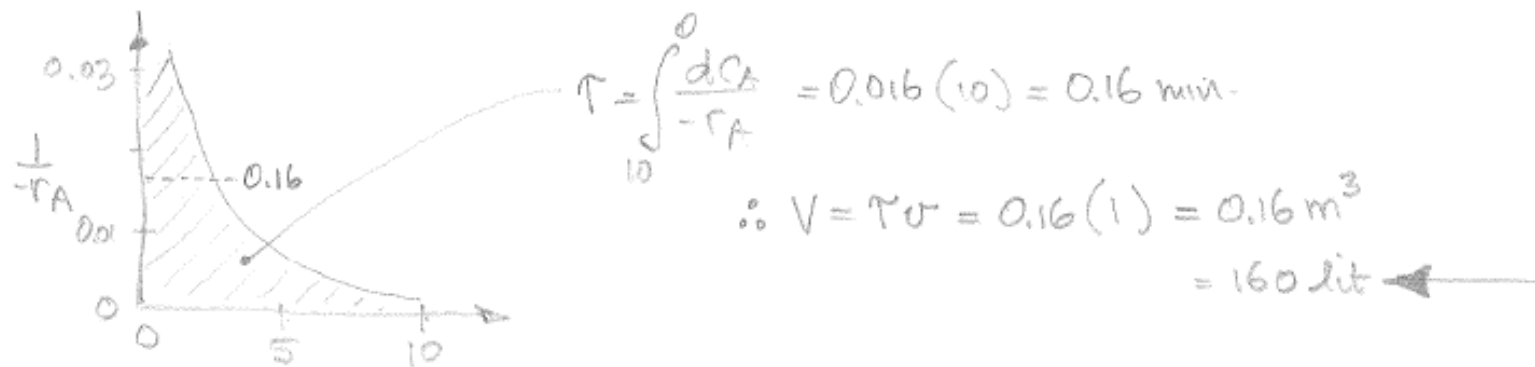
7.19 First find the  $\phi$  vs  $C_A$  curve, then decide which reactor type to use

$C_A$	$\phi(T/A) = \frac{C_A^2}{16C_A^{1/2} + 12C_A + C_A^2}$	$-\frac{1}{r_A} = \frac{1}{16C_A^{1/2} + 12C_A + C_A^2}$
10	0.37	0.0037
9	0.34	0.0042
4	0.167	0.0104
1	0.03	0.03
0.1		0.16

Now plot



Next, to find  $\tau$  plot  $-\frac{1}{r_A}$  vs  $C_A$



The stoichiometry of a liquid-phase decomposition is known to be



In a series of steady-state flow experiments ( $C_{A0} = 100$ ,  $C_{R0} = C_{S0} = 0$ ) in a laboratory mixed flow reactor the following results are obtained:

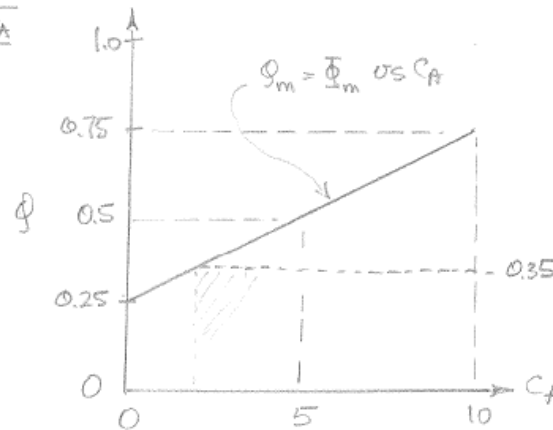
$C_A$	90	80	70	60	50	40	30	20	10	0
$C_R$	7	13	18	22	25	27	28	28	27	25

Further experiments indicate that the level of  $C_R$  and  $C_S$  have no effect on the progress of the reaction.

**7.21.** With  $C_{A0} = 100$  and  $C_{Af} = 20$ , find  $C_R$  at the exit from a mixed flow reactor.

7.21 First let us calculate  $\phi$ , the instantaneous fractional yield. This is obtained directly from the mixed flow run because  $\phi_m = \bar{\phi}_m$

$C_{A0}$	$C_A$	$C_R$	$\phi = \bar{\phi} = \frac{C_R}{C_{A0} - C_A}$
100	90	7	$7/10 = 0.7$
100	80	13	0.65
100	70	18	0.60
100	60	22	0.55
100	50	25	0.50
100	40	27	0.45
100	30	28	0.40
100	20	28	0.35
100	10	27	0.30
100	0	25	$25/100 = 0.25$

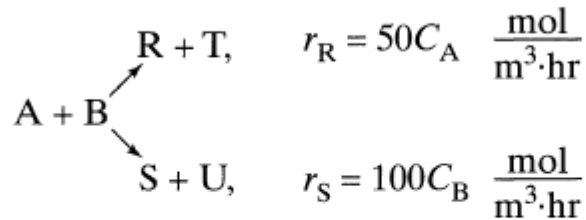


So for mixed flow with  $C_{A0} = 100$

$$C_{Rf} = \bar{\phi}(-\Delta C_A) = \phi(-\Delta C_A) = 0.35(100 - 20) = 28$$

7.23. in a mixed flow reactor;

When aqueous A and aqueous B ( $C_{A0} = C_{B0}$ ) are brought together they react in two possible ways:



to give a mixture whose concentration of active components (A, B, R, S, T, U) is  $C_{\text{total}} = C_{A0} + C_{B0} = 60 \text{ mol/m}^3$ . Find the size of reactor needed and the R/S ratio produced for 90% conversion of an equimolar feed of  $F_{A0} = F_{B0} = 300 \text{ mol/hr}$ :

7.23

$$F_{A0} = 300 \text{ mol/hr}$$

$$C_{A0} = 30 \text{ mol/m}^3$$

$$F_{B0} = 300 \text{ mol/hr}$$

$$C_{B0} = 30 \text{ mol/m}^3$$



$$\phi(R/A) = \frac{50C_A}{50C_A + 100C_B} = \frac{1}{3}$$

$$\phi(S/A) = \frac{100C_B}{50C_A + 100C_B} = \frac{2}{3}$$

$$\therefore C_R = \phi(R/A)(-\Delta C_A) = \frac{1}{3}(30-3) = 9 \text{ mol/m}^3 \quad \therefore R/S = 1/2 \quad \leftarrow$$

$$V = \frac{F_{A0}}{C_{A0}} \cdot \frac{C_{A0} - C_A}{\frac{1}{20}C_A + \frac{1}{10}C_B} = \frac{300}{30} \frac{30-3}{\frac{3}{20} + \frac{3}{10}} = 600 \text{ lit} \quad \leftarrow$$

7.25. in a reactor that gives highest  $C_R$ . Chapter 6 tells that this should be plug flow for A and side entry for B. In such a reactor introduce B in such a way that  $C_B$  is constant throughout the reactor.

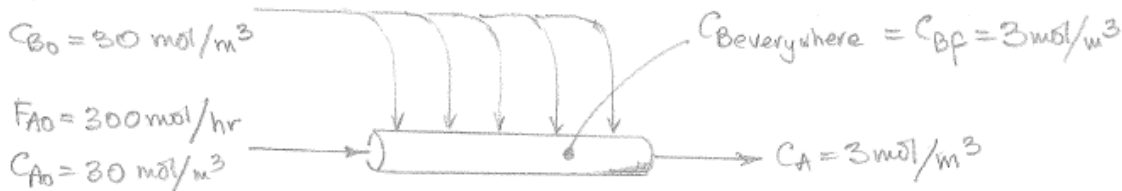
7.25

$$F_{B0} = 300 \text{ mol/hr}$$

$$C_{B0} = 30 \text{ mol/m}^3$$

$$F_{A0} = 300 \text{ mol/hr}$$

$$C_{A0} = 30 \text{ mol/m}^3$$



$$\text{Determine } q(R/A) = \frac{50C_A}{50C_A + 100C_B} = \frac{C_A}{C_A + 2C_B}$$

7.25  
(continued)

$$\therefore C_{Rf} = \int_{C_{Af}}^{C_{A0}} q(R/A) dC_A = \int_3^{30} \frac{C_A}{C_A + 2C_B} dC_A = \left[ C_A - 6 \ln(C_A + 6) \right]_3^{30} = 18.68$$

$$C_{Sf} = \int_{C_{Af}}^{C_{A0}} q(S/A) dC_A = \int_3^{30} \frac{2C_B}{C_A + 2C_B} dC_A = \left[ 6 \ln(C_A + 6) \right]_3^{30} = 8.32$$

$$\text{So } \frac{C_{Rf}}{C_{Sf}} = \frac{18.68}{8.32} \approx 2.25$$

$$\text{Finally } V = \frac{F_{A0}}{C_{A0}} \int_{C_{Af}}^{C_{A0}} \frac{dC_A}{-r_A} = \frac{300}{30} \int_3^{30} \frac{dC_A}{50C_A + 100(3)} = \left[ (10) \left( \frac{1}{50} \right) \ln(50C_A + 300) \right]_3^{30}$$

$$= 0.2773 \text{ m}^3 = 277.3 \text{ lit}$$

**Thank you**

