BT209

Bioreaction Engineering

24/03/2023

Design of parallel reaction

Design for multiple reaction

***Single* reaction:** Requires only one rate expression to describe its kinetic behavior

$$A \rightarrow R$$

Criteria: Only volume of reactor (so far it has been discussed)
(objective: **small reactor size)**

✓ **Performance (size) of a reactor was influenced by the pattern of flow within the vessel (CSTR, PFR)**

***Multiple* reactions:** Require more than one rate expression

Series $A \rightarrow R \rightarrow S \rightarrow T$

Parallel

$$A \xrightarrow{k_1} R \quad \text{(desired product)}$$
$$A \xrightarrow{k_2} S \quad \text{(unwanted product)}$$

Combination

$$A \rightarrow R \rightarrow S, \quad A \rightarrow T, \quad R \rightarrow U$$

Criteria:

1. Volume of reactor(minimum reactor size)
2. Product Distribution (maximization of desired product) (To minimize the downstream process cost to purify the desired product)

✓ Both the size requirement and the distribution of reaction products are affected by the pattern of flow within the vessel for multiple reaction **?**

Product distribution in multiple reaction

Parallel

$$A \xrightarrow{k_1} R \quad \text{(desired product)} \qquad r_R = \frac{dC_R}{dt} = k_1 C_A^{a_1}$$

$$A \xrightarrow{k_2} S \quad \text{(unwanted product)} \qquad r_S = \frac{dC_S}{dt} = k_2 C_A^{a_2}$$

Relative rates of formation of R and S

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

- **Objective: To increase the ratio of r_R/r_S**

- Here C_A, is the only factor in r_R/r_S ratio 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)

Keep C_A, low throughout the reactor by

1) using a mixed flow reactor
2) maintaining high conversions,
3) increasing inert in the feed,
4) decreasing the pressure in gas-phase systems.

Keep C_A high through out the reactor by

1. using a batch or plug flow reactor,
2. maintaining low conversions,
3. removing inert from the feed, or
4. increasing the pressure in gas phase systems.

Cont..

$$A \xrightarrow{k_1} R \quad \text{(desired product)}$$

$$A \xrightarrow{k_2} S \quad \text{(unwanted product)}$$

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

- ❑ **If $a_1 > a_2$** (desired reaction is of higher order than the unwanted reaction)
- ✓ high concentration of A is desirable
- ✓ **As** a result, a batch or plug flow reactor would favor formation of product R and would require a minimum reactor size.

- ❑ **If $a_1 < a_2$**
- ✓ Need a low concentration of A to favor formation of R.
- ✓ But this would also require large mixed flow reactor.

- ❑ **If $a_1 = a_2$** $\quad \frac{r_R}{r_S} = \frac{dC_R}{dC_S} = \frac{k_1}{k_2} = \text{constant}$

➢ Hence, product distribution is fixed by k_1/k_2 alone and is unaffected by type of reactor used.

Cont…

$$A \xrightarrow{k_1} R \quad \text{(desired product)}$$

$$A \xrightarrow{k_2} S \quad \text{(unwanted product)}$$

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

- Product distribution may also control by varying ***k_1/k_2*.** 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.

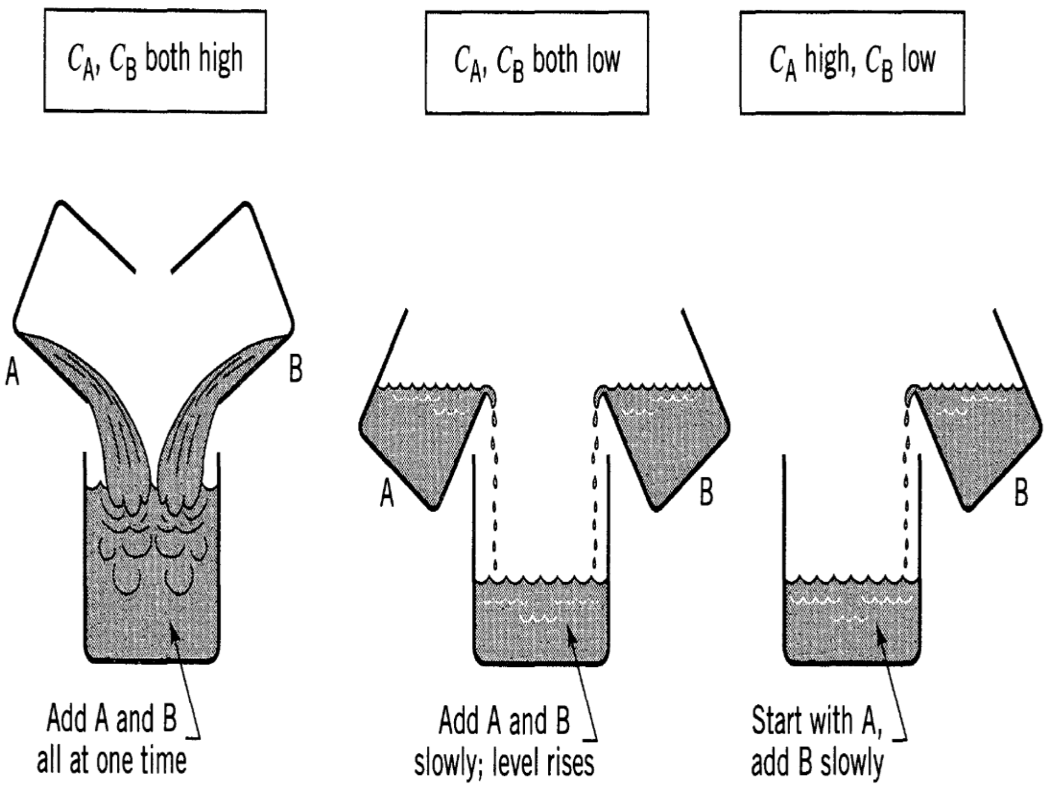
- 2. By using a catalyst. One of the most important features of a catalyst is its selectivity in depressing or accelerating specific reactions.

Control of concentration of reactants for multiple reactants

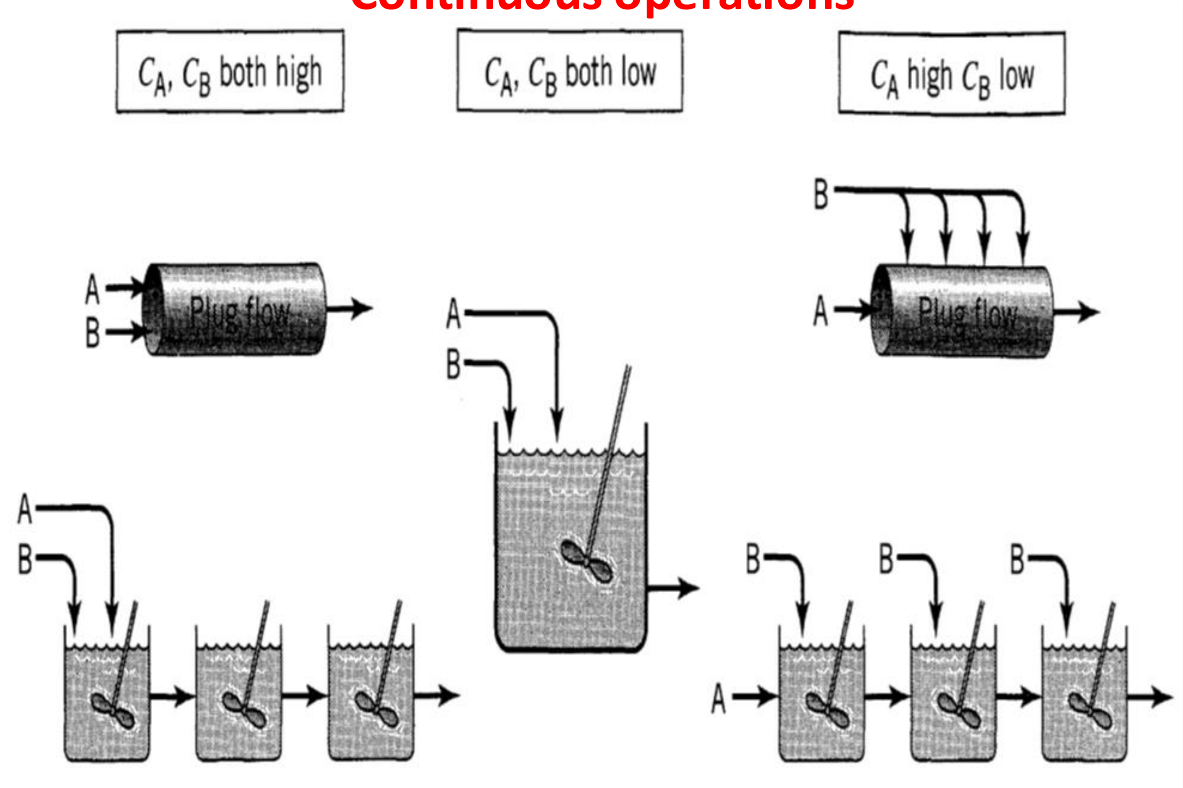
For two or more reactants, combinations of high and low reactant concentrations can be obtained by

- controlling the concentration of feed materials, by having certain components in excess,
- and by using the correct contacting pattern of reacting fluids.

Noncontinuous operations



Continuous operations



- **In any case, the use of the proper contacting pattern is the critical factor in obtaining a favorable distribution of products for multiple reactions**

Quantitative analysis of Product Distribution and Reactor Size

If rate equations are known for the individual reactions,
- ✓ can quantitatively determine product distribution
- ✓ and reactor-size requirements.

$$A \xrightarrow{k_1} R \quad \text{(desired product)}$$
$$A \xrightarrow{k_2} S \quad \text{(unwanted product)}$$

φ = fraction of A disappearing at any instant which is transformed into desired product R.

***Instantaneous fractional yield of* R**

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

For any particular set of reactions and rate equations
- ➢ φ is a function of *CA*,
- ➢ C_A in general varies through the reactor, φ will also change with position in the reactor (in ideal PFR).

Therefore one more parameter: *Overall fractional yield*

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

Φ :fraction of all the reacted A that has been converted into R

✓ **The overall fractional yield is then the mean of the instantaneous fractional yields at all points within the reactor**

Cont…

- Proper averaging for φ depends on
  - the type of flow within the reactor.

- Therefore for plug *flow,* where C_A changes progressively through the reactor

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

Subscript *P* for PFR

- For mixed *flow,* the composition is C_A everywhere, so φ s likewise constant throughout the reactor

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

C_{Af}: outlet concentration of A

Subscript *m* for Mixed flow (CSTR)

Overall Yield for N-number of CSTR in series

For a series of 1, 2, . . . , N mixed flow reactors in which the concentration of A is C_{A1}, C_{A2}, . . . , C_{AN},

Overall yield?

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

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

Product distribution (graphical) in different reactors

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

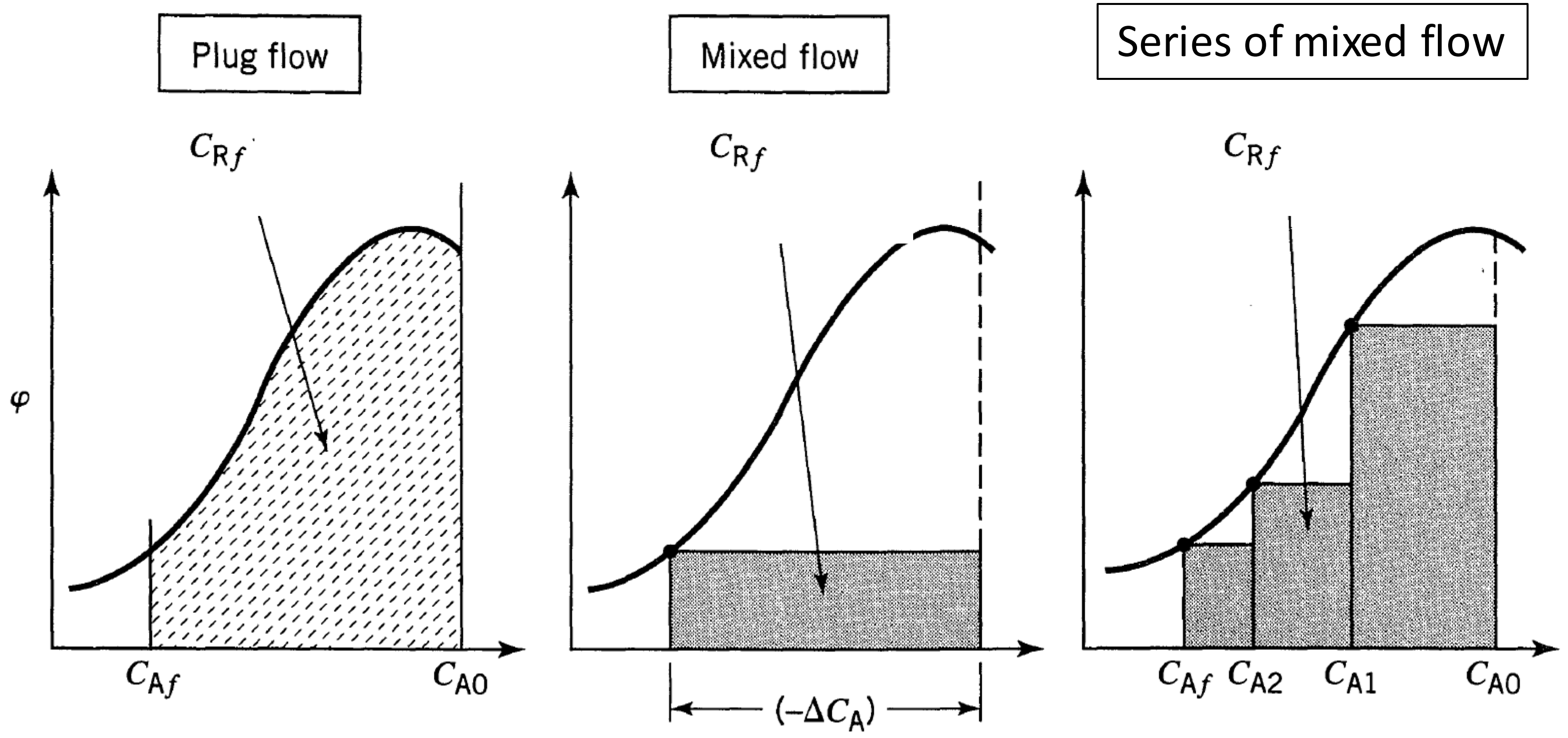
For MFR: $$\Phi_m = \varphi_{\text{evaluated at } C_{Af}}$$

$A \xrightarrow{k_1} R$ (desired product)

$A \xrightarrow{k_2} S$ (unwanted product)

- **For any reactor**

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

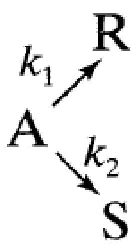


Choose of reactor (flow pattern) for different shape of φ for best production of R

➢ **Shape of the φ versus C_A curve determines which type of flow gives the best product distribution**

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

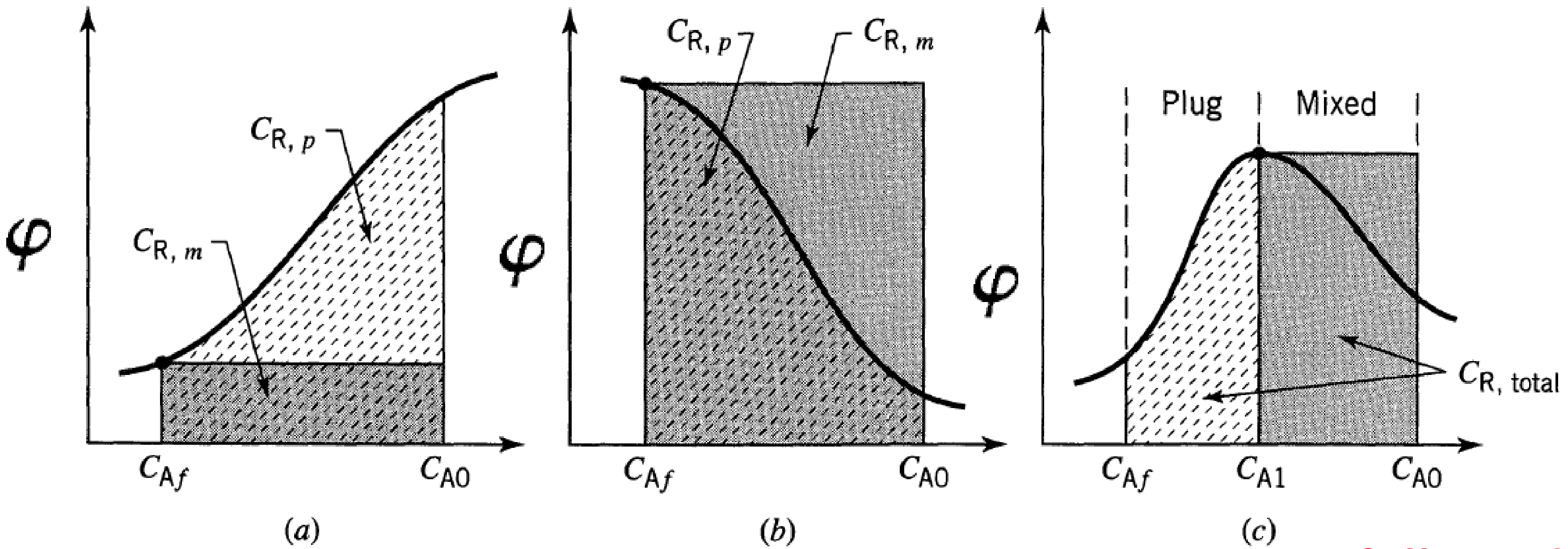
For MFR: $$\Phi_m = \varphi_{\text{evaluated at } C_{Af}}$$



➢ **For any reactor**

$$\Phi = \left(\frac{\text{all R formed}}{\text{all A reacted}} \right) = \frac{C_{Rf}}{C_{A0} - C_{Af}}$$

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



PFR best

CSTR best

CSTR upto C_{A1} followed by PFR best

$C_{R,p}$: Total R production in PFR

$C_{R,m}$: Total R production in CSTR

Notation of φ for multiple reactants or products

- For two or more reactants involved

- ✓ **φ(M/N):** instantaneous fractional yield of M, based on the disappearance of N

Selectivity

- Selectivity also used in place of fractional yield for analysis

$$A \xrightarrow{k_1} R \quad \text{(desired product)}$$

$$A \xrightarrow{k_2} S \quad \text{(unwanted product)}$$

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