Chemical Reaction Engineering

Multiple Reactions

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- Reaction Yield
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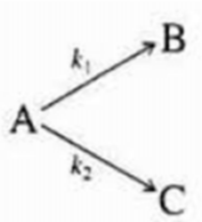
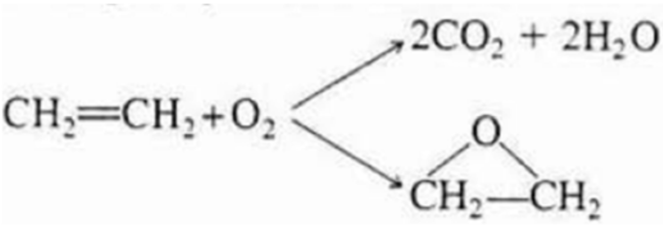
Types of Reactions

Parallel reactions

Are reactions where the reactant is consumed by **two** different reaction pathways to form different products





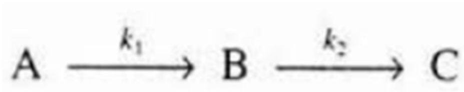
carbon dioxide and water.

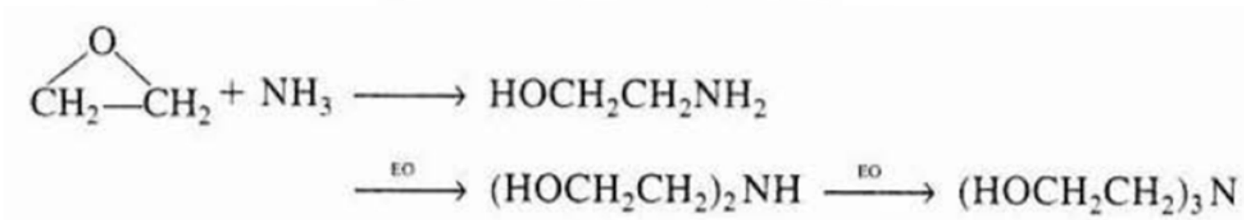
ethylene ethylene oxide

Types of Reactions

Series reactions

Are reactions where the reactant forms an intermediate product, which reacts further to form another product





ethylene oxide ammonia mono-, di-, and triethanolamine

Types of Reactions

Complex reactions

Are multiple reactions that involve a combination of both series and parallel reaction

$$A + B \longrightarrow C + D$$
$$A + C \longrightarrow E$$

$$C_2H_5OH \longrightarrow C_2H_4 + H_2O$$
$$C_2H_5OH \longrightarrow CH_3CHO + H_2$$
$$C_2H_4 + CH_3CHO \longrightarrow C_4H_6 + H_2O$$

Types of Reactions

Independent reactions

Are reactions that occur at the same time but neither products nor reactants react with themselves or one another

$$A \longrightarrow B + C$$
$$D \longrightarrow E + F$$

crude oil

$$C_{15}H_{32} \longrightarrow C_{12}C_{26} + C_3H_6$$
$$C_8H_{18} \longrightarrow C_6H_{14} + C_2H_4$$

Types of Reactions

Desired and Undesired Reactions

- Of particular interest are reactants that are consumed in the formation of a *desired product,* D, and the formation of an *undesired product,* U, in a competing or side reaction.

In the parallel reaction sequence

$$A \xrightarrow{k_D} D$$
$$A \xrightarrow{k_U} U$$

Or in the series sequence

$$A \xrightarrow{k_D} D \xrightarrow{k_U} U$$

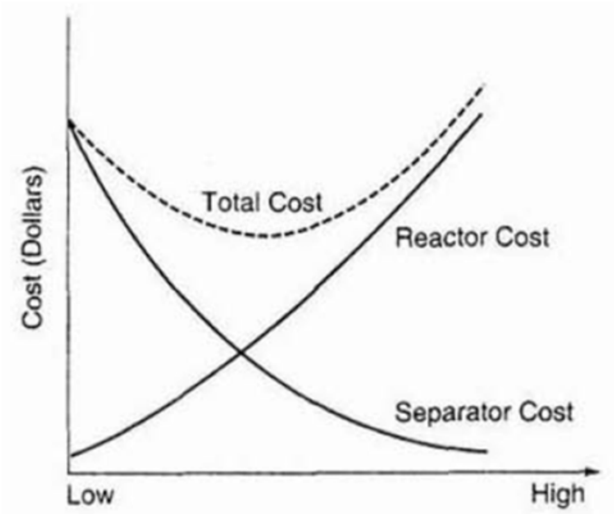
- In such reactions, the target is to minimize the formation of U and maximize *the* formation of D.

Selectivity

- Tells us how one product is favored over another when we have multiple reactions.
- The instantaneous selectivity of D with respect to U

$$S_{D/U} = \frac{r_D}{r_U} = \frac{\text{rate of formation of D}}{\text{rate of formation of U}}$$

- $S_{D/U}$ is an important parameter for the design and selection of our reaction system to maximize the selectivity.



Efficiency of a reactor system.

- In terms of the flow rates leaving the reactor, overall selectivity is

$$\tilde{S}_{D/U} = \frac{F_D}{F_U} = \frac{\text{Exit molar flow rate of desired product}}{\text{Exit molar flow rate of undesired product}}$$

Selectivity

- For a batch reactor, the overall selectivity is given in terms of moles of D and U *at* the end of the reaction time

$$\tilde{S}_{D/U} = \frac{N_D}{N_U}$$

Example

Develop a relationship between $S_{D/U}$ and $\tilde{S}_{D/U}$ for a CSTR.

$$A \xrightarrow{k_D} D \qquad S_{D/U} = \frac{r_D}{r_U}$$

$$A \xrightarrow{k_U} U \qquad \tilde{S}_{D/U} = \frac{F_D}{F_U}$$

A mole balance on D for a CSTR yields

$$F_D = r_D V$$

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Example cont.

a mole balance on U yields $F_U = r_U V$

$$\tilde{S}_{D/U} = \frac{F_D}{F_U} = \frac{r_D V}{r_U V} = \frac{r_D}{r_U} = S_{D/U}$$

for a CSTR the overall and instantaneous selectivities are equal.

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Reaction Yield

- The yield at a point can be defined as the ratio of the reaction rate of a given product to the reaction rate of the key reactant

$$Y_D = \frac{r_D}{-r_A}$$

- The overall yield, is defined as the ratio of moles of product formed *at* the end of the reaction to the number *of* moles of the key reactant

For a batch system $$\tilde{Y}_D = \frac{N_D}{N_{A0} - N_A}$$

For a flow system $$\tilde{Y}_D = \frac{F_D}{F_{A0} - F_A}$$

- As with selectivity, the instantaneous yield and the overall yield are identical for a CSTR

Parallel Reactions

In such system, targets are

- Minimizing the undesired product, U, through the selection of reactor type and conditions.
- Development of efficient reactor schemes

For the competing reactions

$$A \xrightarrow{k_D} D \quad \text{(desired)} \qquad r_D = k_D C_A^{\alpha_1}$$

$$A \xrightarrow{k_U} U \quad \text{(undesired)} \qquad r_U = k_U C_A^{\alpha_2}$$

where α_1 and α_2 are positive reaction orders.

- The rate of disappearance of **A** for this reaction sequence is the sum of the rates of formation of U and D:

$$-r_A = r_D + r_U$$

Parallel Reactions

$$-r_A = k_D C_A^{\alpha_1} + k_U C_A^{\alpha_2}$$

$$\Rightarrow \quad S_{DU} = \frac{r_D}{r_U} = \frac{k_D}{k_U} C_A^{\alpha_1 - \alpha_2}$$

Maximizing the Desired Product for One Reactant

Case 1: $\alpha_1 > \alpha_2$

$$\Rightarrow \quad \alpha_1 - \alpha_2 = a > 0$$

$$S_{D/U} = \frac{r_D}{r_U} = \frac{k_D}{k_U} C_A^{a}$$

Parallel Reactions

- To make this ratio as large as possible. we want to *carry* out the reaction in a manner that will keep the concentration of reactant A as high as possible, during the reaction.
  - If the reaction is carried out in the gas phase run it without inserts and at high pressures.
  - If the reaction is in the liquid phase, the use of diluents should be kept to a minimum
  - A batch or plug-flow reactor should be used in this case because, in these two reactors, the concentration of A starts at a high value and drops progressively during the course of the reaction.
  - In a CSTR, the concentration of reactant within the reactor is always at its lowest value

Case 2: $\alpha_2 > \alpha_1$

$$A \xrightarrow{k_D} D \quad \text{(desired)} \qquad r_D = k_D C_A^{\alpha_1}$$

$$A \xrightarrow{k_U} U \quad \text{(undesired)} \qquad r_U = k_U C_A^{\alpha_2}$$

Parallel Reactions

Let $b = \alpha_2 - \alpha_1$, where b is a positive number:

$$S_{D/U} = \frac{r_D}{r_U} = \frac{k_D C_A^{\alpha_1}}{k_U C_A^{\alpha_2}} = \frac{k_D}{k_U C_A^{\alpha_2-\alpha_1}} = \frac{k_D}{k_U C_A^{b}}$$

For the ratio r_D/r_U to be high, the concentration of A should be as low as possible.

- Diluting the feed with inserts and running the reactor at low concentration of A
- A CSTR should *be* used because the concentrations of reactants are maintained at a low level
- A recycle reactor in which the product stream acts as a diluent could be used to maintain the entering concentrations of A at a low value.

Parallel Reactions

Case 3: $E_D > E_U$

- *In this* case the specific reaction rate of the desired reaction k_D (and therefore the overall rate r_D) increases more rapidly with increasing temperature than does the specific rate of the undesired reaction k_U.
- Consequently, the reaction system should be operated at the highest possible temperature to maximize S_{DU}

Case 4: $E_U > E_D$

- *In this* case *the* reaction should be carried out at a low temperature to maximize S_{DU} but not so low that the desired reaction does not proceed to any significant extent

Example

Reactant A decomposes by three simultaneous reactions to form three produc one that is desired, B, and two that are undesired, X and Y. These gas-pha reactions, along with the appropriate rate laws, are called the Trambouze rea tions [*AIChE J.* 5, 384 (1959)].

$$1)\quad A \xrightarrow{k_1} X \qquad -r_{1A} = r_X = k_1 \quad = 0.0001 \frac{\text{mol}}{\text{dm}^3 \cdot \text{s}}$$

$$2)\quad A \xrightarrow{k_2} B \qquad -r_{2A} = r_B = k_2 C_A = (0.0015\ s^{-1}) C_A$$

$$3)\quad A \xrightarrow{k_3} Y \qquad -r_{3A} = r_Y = k_3 C_A^2 = 0.008 \frac{\text{dm}^3}{\text{mol} \cdot \text{s}} C_A^2$$

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Example Cont.

The specific reaction rates are given at 300 K and the activation energies for reacti (1), (2), and (3) are E_1 = 10,000 kcal/mole, E_2 = 15,000 kcal/mole, and E_3 = 20,0 kcal/mole. How and under what conditions (e.g., reactor type(s), temperature, conc trations) should the reaction be carried out to maximize the selectivity of B for entering concentration of A of 0.4*M* and a volumetic flow rate of 2.0 dm³/s.

Example Cont.

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Example Cont.

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Reactor Selection and Operating Conditions

- Considering the two simultaneous reactions

$$A + B \xrightarrow{k_1} D \qquad r_D = k_1 C_A^{\alpha_1} C_B^{\beta_1}$$

$$A + B \xrightarrow{k_2} U \qquad r_U = k_2 C_A^{\alpha_2} C_B^{\beta_2}$$

The rate selectivity parameter

$$S_{D/U} = \frac{r_D}{r_U} = \frac{k_1}{k_2} C_A^{\alpha_1 - \alpha_2} C_B^{\beta_1 - \beta_2}$$

- **Reactor Selection Criteria are**: Selectivity, Yield, Temperature, control, Safety and Cost

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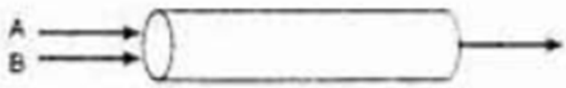
Reactor Selection and Operating Conditions

Case I: $\alpha_1 > \alpha_2$, $\beta_1 > \beta_2$. Let $a = \alpha_1 - \alpha_2$ and $b = \beta_1 - \beta_2$,

where a and b are positive constants

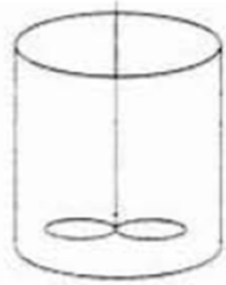
$$S_{D/U} = \frac{r_D}{r_U} = \frac{k_1}{k_2} C_A^a C_B^b$$

To maximize the ratio r_D/r_U, maintain the concentrations of both A and B as high as possible.



A tubular reactor

A batch reactor



High pressures (if gas phase), and reduce inerts

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Reactor Selection and Operating Conditions

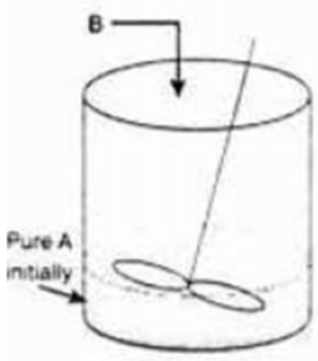
Case II: $\alpha_1 > \alpha_2$, $\beta_1 < \beta_2$. Let $a = \alpha_1 - \alpha_2$ and $b = \beta_2 - \beta_1$

where a and b are positive constants

$$S_{D/U} = \frac{r_D}{r_U} = \frac{k_1 C_A^a}{k_2 C_B^b}$$

Make the concentration of A high and the concentration of B low, thus use

i. A semi-batch reactor in which B is fed slowly into a large amount of A



(d) Semibatch

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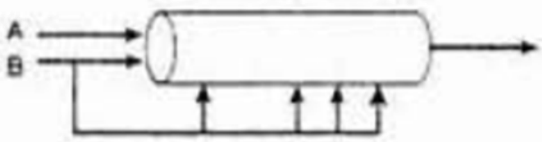
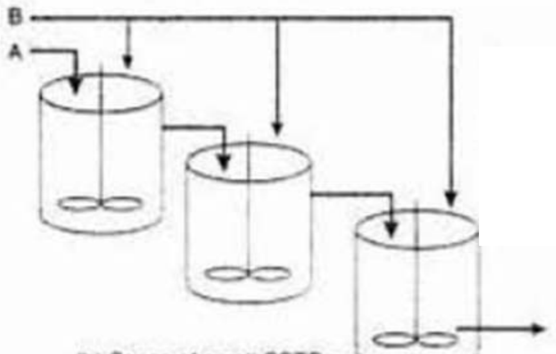
Reactor Selection and Operating Conditions

ii. A membrane reactor or a tubular reactor with side streams of B continuously fed to the reactor



(f) A membrane reactor or a tubular reactor with side streams

iii. A series of small CSTRs with A fed only to the first reactor and small amounts of *B* fed to each reactor. In this way B is mostly consumed before the CSTR exit stream flows into the next reactor



(h) Series of small CSTRs

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Reactor Selection and Operating Conditions

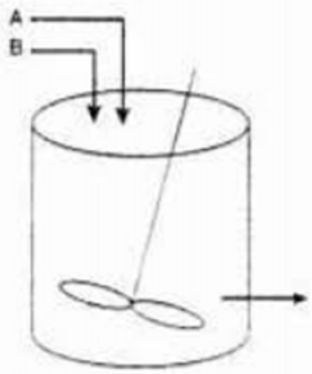
Case III: $\alpha_1 < \alpha_2$, $\beta_1 < \beta_2$. Let $a = \alpha_2 - \alpha_1$ and $b = \beta_2 - \beta_1$,

where a and b are positive constants

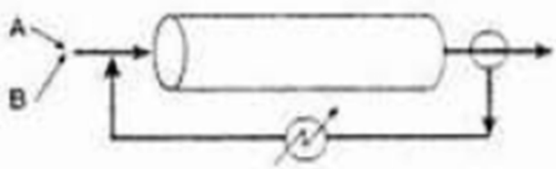
$$S_{D/U} = \frac{r_D}{r_U} = \frac{k_1}{k_2 C_A^a C_B^b}$$

To make $S_{D/U}$ as large as possible, the reaction should be carried out at low centrations of A and of B. Use

i. A CSTR



ii. A tubular reactor in which there is a large recycle ratio



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Reactor Selection and Operating Conditions

iii. A feed diluted with inserts

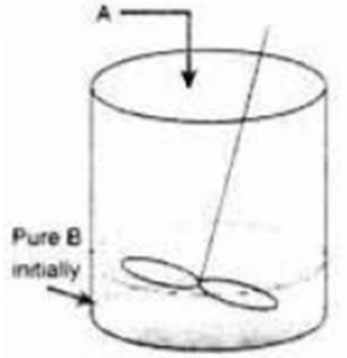
iv. Low pressure (if gas phase)

Case IV: $\alpha_1 < \alpha_2$, $\beta_1 > \beta_2$. Let $a = \alpha_2 - \alpha_1$ and $b = \beta_1 - \beta_2$.

$$S_{D/U} = \frac{r_D}{r_U} = \frac{k_1 C_B^b}{k_2 C_A^a}$$

To maximize $S_{D/U}$, run the reaction at high concentrations of B and low concentrations of A. Use

i. A semi-batch reactor with A slowly fed to a large amount of B



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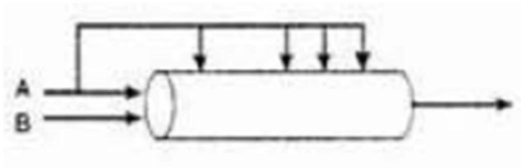
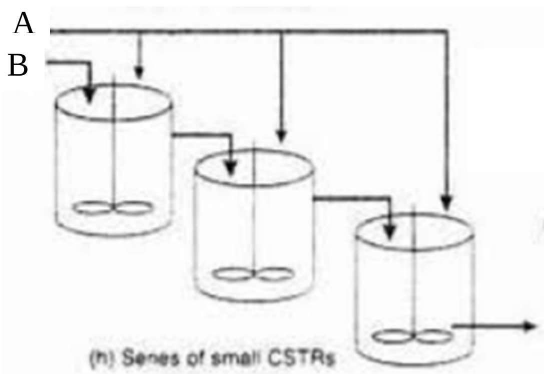
Reactor Selection and Operating Conditions

ii. A membrane reactor or a tubular reactor with side streams of A



iii. A series of small CSTRs with fresh A fed to each reactor



(h) Series of small CSTRs

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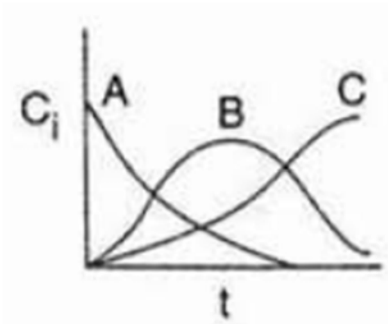
Series Reactions

- For series of consecutive reactions, the most important variable is time: space-time: for a flow reactor and real-time for a batch reactor

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

Assuming species B is the desired product



- If the first reaction is slow and the second reaction is Fast, it will be extremely difficult to produce species B.
- If the first reaction (formation of B) is fast and the reaction to form *C* is slow, a large yield *of* B *can* be achieved.
- If the reaction is allowed to proceed for a long time in a batch reactor, or if the tubular reactor is too long, the desired product B will be converted to the undesired product *C.*

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Example

The oxidation of ethanol to form acetaldehyde is carried out on a catalyst of 4 wt % Cu–2 wt % Cr on Al_2O_3.[3] Unfortunately, acetaldehyde is also oxidized on this catalyst to form carbon dioxide. The reaction is carried out in a threefold excess of oxygen and in dilute concentrations (ca. 0.1% ethanol, 1% O_2, and 98.9% N_2). Consequently, the volume change with the reaction can be neglected. Determine the concentration of acetaldehyde as a function of space-time,

$$CH_3CH_2OH(g) \xrightarrow[-H_2O]{+\frac{1}{2}O_2} CH_3CHO \xrightarrow[-2H_2O]{+\frac{5}{2}O_2} 2CO_2$$

The reactions are irreversible and first order in ethanol and acetaldehyde, respectively.

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Example Cont.

Example Cont.

Example Cont.

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Example Cont.

Example Cont.

Example Cont.

Net Rates of Reaction

- To sum up the rates of formation for each reaction in order to obtain the net rate of formation

$$\text{Reaction 1:} \quad A + B \xrightarrow{k_{1A}} 3C + D$$

$$\text{Reaction 2:} \quad A + 2C \xrightarrow{k_{2A}} 3E$$

$$\text{Reaction 3:} \quad 2B + 3E \xrightarrow{k_{3B}} 4F$$

$$\vdots$$

$$\text{Reaction } q\text{:} \quad E + 2F \xrightarrow{k_{qE}} G$$

$$r_A = r_{1A} + r_{2A} + r_{3A} + \cdots + r_{qA} = \sum_{i=1}^{q} r_{iA}$$

$$r_B = r_{1B} + r_{2B} + r_{3B} + \cdots + r_{qB} = \sum_{i=1}^{q} r_{iB}$$

Net Rates of Reaction

In general the net rate of reaction for species *j* is the sum of all rates of the reactions in which species *j* appears.

For *q* reactions taking place,

$$r_j = \sum_{i=1}^{q} r_{ij}$$

$$r_{ij} = k_{ij} f_i(C_A, C_B \cdots C_j \cdots C_n)$$

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Net Rates of Reaction

Reaction (1): $A + B \xrightarrow{k_{1A}} 3C + D$ $\quad -r_{1A} = k_{1A} C_A C_B$

Reaction (2): $A + 2C \xrightarrow{k_{2A}} 3E$ $\quad -r_{2A} = k_{2A} C_A C_C^2$

or in terms of the rates of formation of A

In Reaction 1: $r_{1A} = -k_{1A} C_A C_B$

In Reaction 2: $r_{2A} = -k_{2A} C_A C_C^2$

the net rate of formation of A

$$r_A = r_{1A} + r_{2A} = -k_{1A} C_A C_B - k_{2A} C_A C_C^2$$

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Stoichiometry: Relative Rates of Reaction

- For the reaction $aA + bB \longrightarrow cC + dD$

$$\frac{-r_A}{a} = \frac{-r_B}{b} = \frac{r_C}{c} = \frac{r_D}{d}$$

- In working with multiple reactions, it is usually more advantageous to relate the rates *of formation* of each species to one another

for reaction i

$$\frac{r_{iA}}{-a_i} = \frac{r_{iB}}{-b_i} = \frac{r_{iC}}{c_i} = \frac{r_{iD}}{d_i}$$

Reaction (1): $A + B \xrightarrow{k_{1A}} 3C + D$ Given: $r_{1A} = -k_{1A}C_AC_B$

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Stoichiometry: Relative Rates of Reaction

$$\frac{r_{1A}}{-1} = \frac{r_{1B}}{-1} = \frac{r_{1C}}{3} = \frac{r_{1D}}{1}$$

$$r_{1B} = r_{1A} = -k_{1A}C_AC_B$$

$$r_{1C} = 3(-r_{1A}) = 3k_{1A}C_AC_B$$

$$r_{1D} = -r_{1A} = k_{1A}C_AC_B$$

for Reaction 2,

Reaction (2): $A + 2C \xrightarrow{k_{2A}} 3E$ Given: $r_{2A} = -k_{2A}C_AC_C^2$

$$\frac{r_{2A}}{-1} = \frac{r_{2C}}{-2} = \frac{r_{2E}}{3}$$

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Stoichiometry: Relative Rates of Reaction

the rate of formation of species *E* in reaction 2, r_{2E}, is

$$r_{2E} = \frac{3}{-1}(r_{2A}) = -3(-k_{2A}C_A C_C^2) = 3k_{2A}C_A C_C^2$$

and the rate of formation of C in reaction 2 is

$$r_{2C} = \frac{-2}{-1} r_{2A} = -2k_{2A}C_A C_C^2$$

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Stoichiometry: Net Rates of Reaction

- For the reactions

(1) $\quad A + B \xrightarrow{k_{1A}} 3C + D$

(2) $\quad A + 2C \xrightarrow{k_{2A}} 3E$

the net rates of reaction for species A, B, C, D, and E are

$$r_A = r_{1A} + r_{2A} = -k_{1A}C_A C_B - k_{2A}C_A C_C^2$$
$$r_B = r_{1B} = -k_{1A}C_A C_B$$
$$r_C = r_{1C} + r_{2C} = 3k_{1A}C_A C_B - 2k_{2A}C_A C_C^2$$
$$r_D = r_{1D} = k_{1A}C_A C_B$$
$$r_E = r_{2E} = 3k_{2A}C_A C_C^2$$

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Example

Reaction 1: $4NH_3 + 6NO \longrightarrow 5N_2 + 6H_2O \quad -r_{1NO} = k_{1NO} C_{NH_3} C_{NO}^{1.5}$

Reaction 2: $2NO \longrightarrow N_2 + O_2 \quad r_{2N_2} = k_{2N_2} C_{NO}^2$

Reaction 3: $N_2 + 2O_2 \longrightarrow 2NO_2 \quad -r_{3O_2} = k_{3O_2} C_{N_2} C_{O_2}^2$

Write the rate law for each species in each reaction and then write the net rates formation of NO, O_2, and N_2.

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Example Cont.

Stoichiometry: Concentrations

$$C_j = \frac{F_j}{v_0}$$

For ideal gases
$$C_j = \frac{F_{T0}}{v_0}\left(\frac{F_j}{F_T}\right)\frac{P}{P_0}\frac{T_0}{T} = C_{T0}\left(\frac{F_j}{F_T}\right)\frac{P}{P_0}\frac{T_0}{T}$$

where
$$F_T = \sum_{j=1}^{n} F_j \qquad \text{and} \qquad C_{T0} = \frac{P_0}{RT_0}$$

For isothermal systems ($T = T_0$) with no pressure drop ($P = P_0$)

$$C_j = C_{T0}\left(\frac{F_j}{F_T}\right)$$

Multiple Reactions in a PFR/PBR

$$\frac{dF_1}{dV} = r_1 = \sum_{i=1}^{m} r_{i1} = \text{fn}_1\left(C_{T0}\frac{F_1}{F_T}, \ldots, C_{T0}\frac{F_j}{F_T}\right)$$

$$\frac{dF_j}{dV} = r_j = \sum_{i=1}^{q} r_{ij} = \text{fn}_j\left(C_{T0}\frac{F_1}{F_T}, \ldots, C_{T0}\frac{F_j}{F_T}\right)$$

Example

Write the mole balances on a PFR **in** terms of molar flow rates for each species.

Reaction 1: $4NH_3 + 6NO \longrightarrow 5N_2 + 6H_2O \quad -r_{1NO} = k_{1NO}C_{NH_3}C_{NO}^{1.5}$

Reaction 2: $2NO \longrightarrow N_2 + O_2 \quad r_{2N_2} = k_{2N_2}C_{NO}^{2}$

Reaction 3: $N_2 + 2O_2 \longrightarrow 2NO_2 \quad -r_{3O_2} = k_{3O_2}C_{N_2}C_{O_2}^{2}$

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Example Cont.

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Example Cont.

Example Cont.

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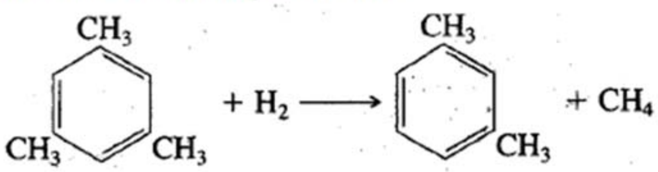
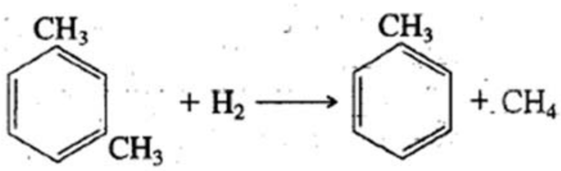
Example

The production of m-xylene by the hydrodealkylation of mesitylene over a Houdry Detrol catalyst[5] involves the following reactions:



$$-r_{1M} = k_1 C_M C_H^{0.5}$$

m-Xylene can also undergo hydrodealkylation to form toluene:



$$r_{2T} = k_2 C_X C_H^{0.5}$$

where the subscripts are: M = mesitylene, X = m-xylene, T = toluene, Me = methane, and H = hydrogen (H_2).

The second reaction is undesirable, because m-xylene sells for a higher price than toluene (65 cents/lb vs. 11.4 cents/lb).[6] Thus we see that there is a significant incentive to maximize the production of m-xylene..

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Example Cont.

The hydrodealkylation of mesitylene is to be carried out isothermally at 1500°R and 35 atm in a packed-bed reactor in which the feed is 66.7 mol% hydrogen and 33.3 mol% mesitylene. The volumetric feed rate is 476 ft^3/h and the reactor volume (i.e., $V = W/\rho_b$) is 238 ft^3.

At 1500°R the specific reaction rates are:

Reaction 1: $k_1 = 55.20\ (ft^3/lb\ mol)^{0.5}/h$

Reaction 2 $k_2 = 30.20\ (ft^3/lb\ mol)^{0.5}/h$

The bulk density of the catalyst has been included in the specific reaction rate (i.e., $k_1 = k_1'\rho_b$).

Plot the concentrations of hydrogen, mesitylene, and xylene as a function of space-time. Calculate the space-time where the production of xylene is a maximum (i.e., τ_{opt}).

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Example Cont.

Mole Balances:

$$\frac{dF_H}{dV} = r_H \qquad \frac{dF_M}{dV} = r_M \qquad \frac{dF_X}{dV} = r_X \qquad \frac{dF_T}{dV} = r_T$$

$$\frac{dF_{Me}}{dV} = r_{Me}$$

Reaction 1: $M + H \longrightarrow X + Me$ $\qquad -r_{1M} = k_1 C_H^{1/2} C_M$

Reaction 2: $X + H \longrightarrow T + Me$ $\qquad r_{2T} = k_2 C_H^{1/2} C_X$

$$-r_{1H} = -r_{1M} = r_{1Me} = r_{1X}$$

$$r_{2T} = r_{2Me} = -r_{2H} = -r_{2X}$$

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Example Cont.

Net rates:

$$r_M = r_{1M} = -k_1 C_H^{1/2} C_M$$

$$r_H = r_{1H} + r_{2H} = r_{1H} - r_{2T} = -k_1 C_H^{1/2} C_M - k_2 C_H^{1/2} C_X$$

$$r_X = r_{1X} + r_{2X} = -r_{1H} - r_{2T} = k_1 C_H^{1/2} C_M - k_2 C_H^{1/2} C_X$$

$$r_{Me} = r_{1Me} + r_{2Me} = -r_{1H} + r_{2T} = k_1 C_H^{1/2} C_M + k_2 C_H^{1/2} C_X$$

$$r_T = r_{2T} = k_2 C_H^{1/2} C_X$$

Example Cont.

$$v = v_0 \frac{F_T}{F_{T0}} \frac{P_0}{P} \frac{T}{T_0}$$

$P = P_0$ (i.e., $y = 1$), $T = T_0$, and there is no change in the total number of moles;

$$\Rightarrow \quad v = v_0$$

Flow rates:

$$F_H = v_0 C_H \qquad F_M = v_0 C_M \qquad F_X = v_0 C_X$$

$$F_{Me} = v_0 C_{Me} = F_{H0} - F_H = v_0 (C_{H0} - C_H)$$

$$F_T = F_{M0} - F_M - F_X = v_0 (C_{M0} - C_M - C_X)$$

Example Cont.

Combining and substituting in terms of the space-time

$$\tau = \frac{V}{v_0}$$

$$\frac{dC_H}{d\tau} = -k_1 C_H^{1/2} C_M - k_2 C_X C_H^{1/2}$$

$$\frac{dC_M}{d\tau} = -k_1 C_M C_H^{1/2}$$

$$\frac{dC_X}{d\tau} = k_1 C_M C_H^{1/2} - k_2 C_X C_H^{1/2}$$

Parameter evaluation:

At $T_0 = 1{,}500°$ R and $P_0 = 35$ atm, the total concentration is

$$C_{T0} = \frac{P_0}{RT_0} = \frac{35 \text{ atm}}{\left(0.73 \frac{\text{atm ft}^3}{\text{lb mol} \cdot °\text{R}}\right)(1{,}500°\text{R})} = 0.032 \text{ lb mol/ft}^3$$

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Example Cont.

$$C_{H0} = y_{H0} C_{T0} = (0.667)(0.032 \text{ kmol/ft}^3) = 0.021 \text{ lb mol/ft}^3$$

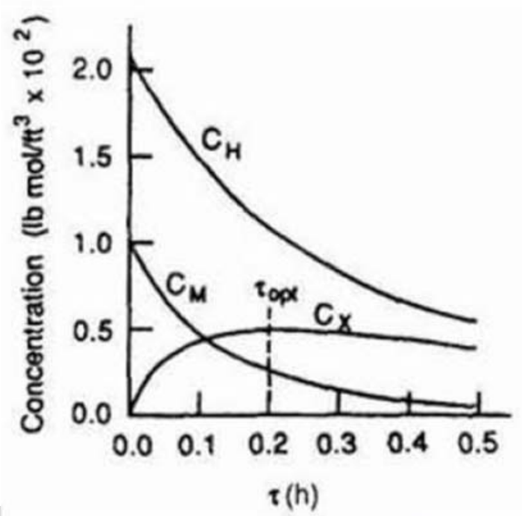
$$C_{M0} = \frac{1}{2} C_{H0} = 0.0105 \text{ lb mol/ft}^3$$

$$C_{X0} = 0$$

$$\tau = \frac{V}{v_0} = \frac{238 \text{ ft}^3}{476 \text{ ft}^3/\text{h}} = 0.5 \text{ h}$$

$$F_{T0} = C_{T0} v_0 = \left(0.032 \frac{\text{lb mol}}{\text{ft}^3}\right)\left(476 \frac{\text{ft}^3}{\text{h}}\right)$$

$$F_{T0} = 15.23 \text{ mol/h}$$



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Multiple Reactions in a CSTR

$$V = \frac{F_{j0} - F_j}{-r_j}$$

Rearranging

$$F_{j0} - F_j = -r_j V$$

Recall that

$$r_j = \sum_{i=1}^{q} r_{ij} = f_j(C_1, C_2, \ldots, C_N)$$

For a CSTR, a coupled set of algebraic equations analogous to PFR differential equations must be solved.

The total molar flow rate for n species is

$$F_T = \sum_{j=1}^{n} F_j$$

Multiple Reactions in a CSTR

For q reactions occurring in the gas phase, where N different species

$$F_{10} - F_1 = -r_1 V = V \sum_{i=1}^{q} -r_{i1} = V \cdot f_1 \left(\frac{F_1}{F_T} C_{T0}, \ldots, \frac{F_N}{F_T} C_{T0} \right)$$

$$F_{j0} - F_j = -r_j V = V \cdot f_j \left(\frac{F_1}{F_T} C_{T0}, \ldots, \frac{F_N}{F_T} C_{T0} \right)$$

$$F_{N0} - F_N = -r_N V = V \cdot f_N \left(\frac{F_1}{F_T} C_{T0}, \ldots, \frac{F_N}{F_T} C_{T0} \right)$$

Example

For the multiple reactions and conditions described in Example 6-7, calculate conversion of hydrogen and mesitylene along with the exiting concentrations mesitylene, hydrogen, and xylene in a CSTR.

$F_A = vC_A = v_0C_A$, etc.

1. **CSTR Mole Balances:**

$$v_0C_{H0} - v_0C_H = r_HV \qquad v_0C_{M0} - v_0C_M = r_MV \qquad v_0C_X = r_XV$$

$$v_0C_T = r_TV \qquad v_0C_{Me} = r_{Me}V$$

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Example Cont.

Combining Equations

$$C_{H0} - C_H = (k_1C_H^{1/2}C_M + k_2C_H^{1/2}C_X)\tau$$

$$C_{M0} - C_M = (k_1C_H^{1/2}C_M)\tau$$

$$C_X = (k_1C_H^{1/2}C_M - k_2C_H^{1/2}C_X)\tau$$

$$f(C_H) = 0 = C_H - C_{H0} + (k_1C_H^{1/2}C_M + k_2C_H^{1/2}C_X)\tau$$

$$f(C_M) = 0 = C_M - C_{M0} + k_1C_H^{1/2}C_M\tau$$

$$f(C_X) = 0 = (k_1C_H^{1/2}C_M - k_2C_H^{1/2}C_X)\tau - C_X$$

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Example Cont.

For a space time of $\tau = 0.5$, the exiting concentrations are $C_H = 0.0089$, $C_M = 0.0029$, and $C_X = 0.0033$. The overall conversion is

$$\text{Hydrogen:} \quad X_H = \frac{F_{H0} - F_H}{F_{H0}} = \frac{C_{H0} - C_H}{C_{H0}} = \frac{0.021 - 0.0089}{0.021} = 0.58$$

$$\text{Mesitylene:} \quad X_M = \frac{F_{M0} - F_M}{F_{M0}} = \frac{C_{M0} - C_M}{C_{M0}} = \frac{0.0105 - 0.0029}{0.0105} = 0.72$$

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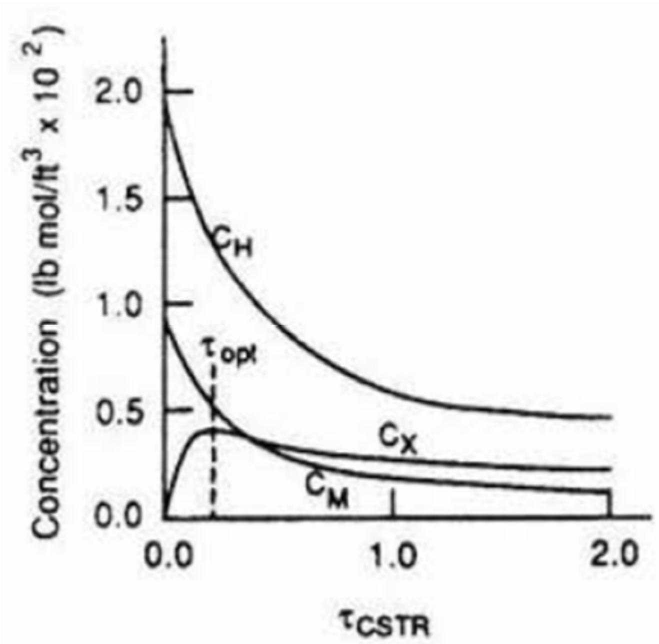
Example Cont.



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