BT209

Bioreaction Engineering

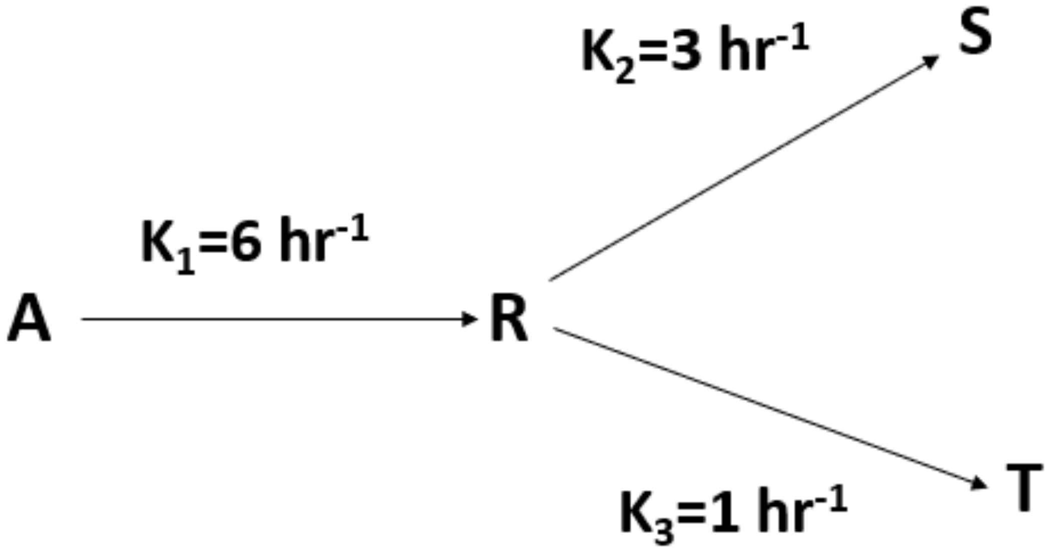
10/04/2023

Problem 1

For the following reactions what reactor type would give the maximum yield of M and estimate roughly the maximum concentration of M. Assume all the reaction are elementary type. [Marks 0.5+0.5]

$A \rightarrow P$	Rate constant: 0.21 s^{-1}
$A \rightarrow M$	Rate constant: 0.20 s^{-1}
$P \rightarrow M$	Rate constant: 4.20 s^{-1}
$M \rightarrow Q$	Rate constant: 0.004 s^{-1}

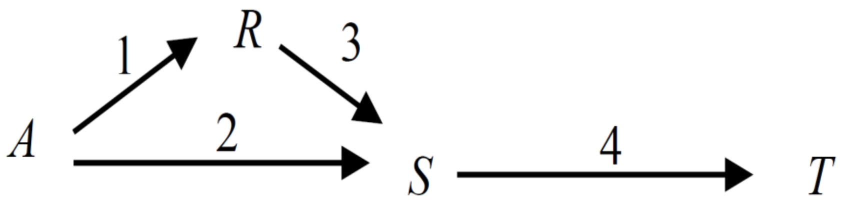
Problem 2



If inlet concentration of A is 1 mol/liter into a PFR, what is the optimum operating condition (space time) to reach maximum concentration of R and what would be the maximum concentration of R? [Marks 0.5+0.5]

Problem 1

With a particular catalyst and at given temperature, the oxidation of A to S proceeds as follows:



$k_1 = 0.21\ s^{-1}$, $k_2 = 0.20\ s^{-1}$, $k_3 = 4.2\ s^{-1}$ and $k_4 = 0.004\ s^{-1}$. What reactor type would give the maximum yield of S. Estimate **roughly** the S^{max} $(C_{A0} = 2\ \mathrm{mol/L})$

solution

$$
\begin{tikzcd}
 & R \arrow[dr, "k_3 = 4.2\ (\text{fast})"] & & \\
A \arrow[ur, "k_1 = 0.21\ (\text{medium})"] \arrow[rr, "k_2 = 0.2\ (\text{medium rate})"'] & & S \arrow[r, "k_4 = 0.004"] & T
\end{tikzcd}
$$

very slow rate.

$$
\begin{tikzcd}
A \arrow[r, bend left, "k_{13} = 0.2"] \arrow[r, "k_2 = 0.2"'] & S \arrow[r] & T
\end{tikzcd}
$$

$$\frac{1}{k_{13}} = \frac{1}{k_1} + \frac{1}{k_3} = \frac{1}{0.2}$$

$$A \xrightarrow{k_{123} = 0.4} S \xrightarrow{k_4 = 0.004} T$$

⇒ Series rxn intermediate S is desired product

∴ use PFR

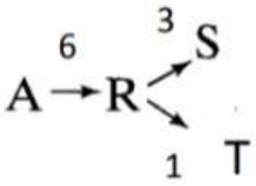
$$\frac{C_S^{max}}{C_{A0}} = \left(\frac{k_{123}}{k_4}\right)^{\frac{k_4}{k_4 - k_{123}}} = 0.955$$

$$\therefore C_S^{max} = 2 \times 0.955 = 1.910 \text{ mol/L}$$

Problem 2

Chemical A reacts to form R ($k_1 = 6\ \text{hr}^{-1}$) and R reacts away to form S ($k_2 = 3\ \text{hr}^{-1}$). In addition R slowly decomposes to form T ($k_3 = 1\ \text{hr}^{-1}$). If a solution containing 1.0 mol/liter of A is introduced into a batch reactor, how long would it take to reach $C_{R,max}$, and what would be $C_{R,max}$?

solution



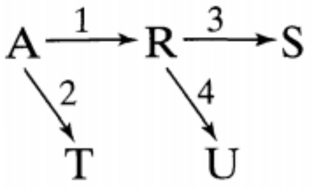
$$t_R^{max} = \frac{ln\left(\frac{k_1}{k_{34}}\right)}{k_1 - k_{34}} = \frac{ln\left(\frac{6}{3+1}\right)}{6-4} = 0.203h = 12.2\ min$$

$$\frac{C_R^{max}}{C_{A0}} = \left(\frac{k_1}{k_{34}}\right)^{\frac{k_{34}}{(k_{34}-k_1)}} = 0.444$$

$$C_R^{max} = 0.444\ mol/l$$

Problem 3

We intend to run the reactions below:



$k_1 = 1.0$ liter/mol·s 2nd order

$k_2 = k_3 = 0.6\ s^{-1}$ 1st order

$k_4 = 0.1$ liter/mol·s 2nd order

in a flow system under the following conditions

Feed flow rate $v = 100$ liters/s

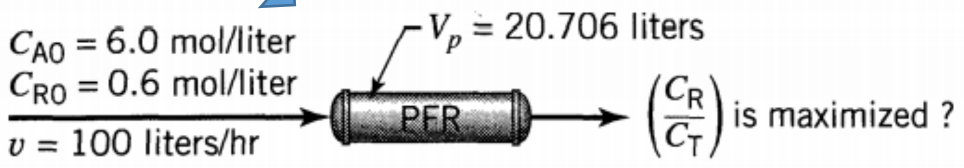
Feed composition $\begin{cases} C_{A0} = 6 \text{ mol/liter} \\ C_{R0} = 0.6 \text{ mol/liter} \end{cases}$

We want to maximize the concentration ratio of CR/CT in the product stream.

As reported (Chem. Eng. Sci., 45, 595-614), the attack on this problem used 2077 continuous variables, 204 integer variables, 2108 constraints, and gave as an optimal solution the design shown in Fig.

(a) Do you think you could do better? If so, what reactor design would you suggest we use, and what C_R/C_T would you expect to obtain?

(b) If you wished to minimize the ratio of C_R/C_T, how would you go about it?



solution

$A \xrightarrow{n=2} R \longrightarrow S$, $A \xrightarrow{n=1} T$, $R \longrightarrow U$

$C_{A0}=6$
$C_{R0}=0.6$
$C_{T0}=0$

The feed has $C_R/C_T=\infty$.

(a) So to maximize C_R/C_T do not react at all
The design of Fig P11 is no good — a)

(b) To minimize C_R/C_T run to completion. All the R will disappear. — b)

Next reaction 1 is second order
reaction 2 is first order
keep C_A low

So use a large MFR, you will end up with most C_T — b)