BT209

Bioreaction Engineering

05/04/2023

Problem 1

Consider the following reactions ($C_{A0} = 10,\ C_{R0} = 0, C_{S0} = 0$) in a mixed flow reactor (CSTR):

$$A \xrightarrow{k_1=1,\ \ n_1=1} R\ \text{(desired product)}\ \xrightarrow{k_2=1,\ \ n_2=0} S$$

(a) Find the operating condition (τ_m) which maximize the C_R in a mixed flow reactor?
(b) At what space time C_R will be non-detectable?

solution

$$A \xrightarrow[n_1=1]{k_1=1} R \xrightarrow[n_2=0]{k_2=1} S$$

$$\boxed{-r_A = -\frac{dC_A}{dt} = k_1 C_A \qquad r_R = \frac{dC_R}{dt} = k_1 C_A - k_2}$$

CSTR

C_A: $\dfrac{\tau_m}{C_{A0}} = \dfrac{C_{A0}-C_A}{C_{A0} \times C_A} \Rightarrow \boxed{\dfrac{C_A}{C_{A0}} = \dfrac{1}{1+k_1\tau_m}}$

C_R: $\dfrac{\tau_m}{C_{R0}} = \dfrac{-C_{R0}+C_R}{C_{R0}(k_1 C_A - k_2)}$

$\Rightarrow \tau_m k_1 C_A - \tau_m k_2 = C_R$

$\Rightarrow \boxed{\dfrac{C_R}{C_{A0}} = \dfrac{k_1\tau_m}{1+k_1\tau_m} - \dfrac{k_2\tau_m}{C_{A0}}}$ for $\tau_m \le \dfrac{C_{A0}}{k_2} - \dfrac{1}{k_1}$

$\tau_m \geq \dfrac{C_{A0}}{k_2} - \dfrac{1}{k_1}$

(b) After that C_R become non-detectable. at $\tau_m = \dfrac{10}{1} - \dfrac{1}{1} = 9$ C_R become non-detectable

$\dfrac{d(C_R/C_{A0})}{d\tau_m} = 0$ for C_R^{max}

$\Rightarrow \dfrac{(1+k_1\tau_m)k_1 - k_1\tau_m \cdot k_1}{(1+k_1\tau_m)^2} - \dfrac{k_2}{C_{A0}} = 0$

$\Rightarrow \dfrac{k_1}{(1+k_1\tau_m)^2} - \dfrac{k_2}{C_{A0}} = 0, \Rightarrow 1+k_1\tau_m = \sqrt{\dfrac{C_{A0}k_1}{k_2}} \Rightarrow \tau_{m,opt} = \sqrt{\dfrac{C_{A0}}{k_1k_2}} - \dfrac{1}{k_1}$

$= \sqrt{10} - 1 = 2.16$

$\boxed{\tau_{m,opt} = 2.162}$ for C_R^{max}

Problem 2

Consider the following elementary reactions ($C_{R0} = 0, C_{S0} = 0$):

$$A \overset{k_1}{\rightarrow} R \text{ (desired product) } \overset{k_2}{\rightarrow} S$$

Derive the maximum C_R in CSTR as

$$C_{R,max} = \frac{C_{Ao}}{\left(1+\sqrt{\frac{k_2}{k_1}}\right)^2}$$

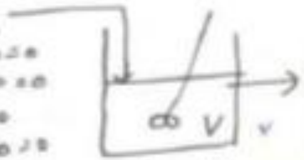
solution

Example: Irreversible first order product distribution in CSTR / PFR ??

$$A \xrightarrow[n=1]{k_1} R \xrightarrow[n=1]{k_2} S$$

CSTR $C_A, C_R, C_S = ??$

C_{A0}, $C_{R0} = 0$, $C_{S0} = 0$, F_{A0}, $F_{R0} = 0$, $F_{S0} = 0$, v_0



C_A, C_R, $C_S = C_{A0} - C_A - C_R$, F_A, F_R, F_S, v

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

Material balance of A

$$F_{A0} = F_A + (-r_A)V$$

$$v C_{A0} = v C_A + k_1 C_A V$$

$$\boxed{\frac{C_A}{C_{A0}} = \frac{1}{1 + k_1 \tau_m}}$$

Material balance of R

$$v C_{R0} = v C_R + (-r_R)V$$

$$0 = v C_R + (-k_1 C_A + k_2 C_R)V$$

$$v C_R + k_2 C_R V = k_1 V \frac{C_{A0}}{1 + k_1 \tau_m} \Rightarrow C_R(v + k_2 V) = \frac{k_1 V C_{A0}}{1 + k_1 \tau_m}$$

$$\frac{C_R}{C_{A0}} = \frac{k_1 V}{(1 + k_1 \tau_m)(v + k_2 V)} = \frac{k_1 \frac{V}{v}}{(1 + k_1 \tau_m)(1 + k_2 \frac{V}{v})} = \frac{k_1 \tau_m}{(1 + k_1 \tau_m)(1 + k_2 \tau_m)}$$

$$\boxed{\frac{C_R}{C_{A0}} = \frac{k_1 \tau_m}{(1 + k_1 \tau_m)(1 + k_2 \tau_m)}}$$

$$C_S = C_{A0} - C_A - C_R$$

$$\frac{C_S}{C_{A0}} = 1 - \frac{1}{1 + k_1 \tau_m} - \frac{k_1 \tau_m}{(1 + k_1 \tau_m)(1 + k_2 \tau_m)}$$

$$\boxed{\frac{C_S}{C_{A0}} = \frac{k_1 k_2 \tau_m^2}{(1 + k_1 \tau_m)(1 + k_2 \tau_m)}}$$

Alternating

$$\frac{\tau_m}{C_{R0}} = \frac{X_R}{r_R} = \frac{C_R - C_{R0}}{C_{A0}(k_1 C_A - k_2 C_R)}$$

KINETICS

$r_A = -k_1 C_A$

$r_R = k_1 C_A - k_2 C_R$

$r_S = k_2 C_R$

$r_A + r_R + r_S = \frac{dC_A}{dt} + \frac{dC_R}{dt} + \frac{dC_S}{dt} = 0$

$C_A + C_R + C_S = C_{A0}$

$C_{R,max} = ??$ and what τ_m will get

$\frac{d}{d\tau_m}(C_R) = 0 \Rightarrow C_{R,max}$ or $\tau_{m,opt}$

$C_R = C_{A0}\frac{K_1\tau_m}{(1+K_1\tau_m)(1+K_2\tau_m)}$

$d\left(\frac{y}{x}\right) = \frac{x\,dy - y\,dx}{x^2}$

$$\frac{dC_R}{d\tau_m} = C_{A0}\left[\frac{(1+K_1\tau_m)(1+K_2\tau_m)K_1 - K_1\tau_m\{K_1(1+K_2\tau_m)+K_2(1+K_1\tau_m)\}}{(1+K_1\tau_m)^2(1+K_2\tau_m)^2}\right]$$

$\Rightarrow (1+K_1\tau_m)(1+K_2\tau_m) = \tau_m K_1(1+K_2\tau_m) + K_2\tau_m(1+K_1\tau_m)$

$\Rightarrow 1+K_1\tau_m + K_2\tau_m + K_1K_2\tau_m^2 = K_1\tau_m + K_1K_2\tau_m^2 + K_2\tau_m + K_1K_2\tau_m^2$

$\Rightarrow 1 = K_1K_2\tau_m^2$

$\Rightarrow \tau_m = \frac{1}{\sqrt{K_1K_2}}$

$$\boxed{\therefore \tau_{m,opt} = \frac{1}{\sqrt{k_1k_2}}}$$

for 1st order series rxn in CSTR

$\frac{dC_A}{dt}$ $\frac{dC_R}{dt}$

$$\therefore\; C_{R,max} = C_{A0}\,\frac{k_1 \tau_{m,opt}}{(1+k_1\tau_{m,opt})(1+k_2\tau_{m,opt})}$$

$$\frac{C_{R,max}}{C_{A0}} = \frac{1}{(1+k_1\tau_{m,opt})\left(\frac{1}{k_1\tau_{m,opt}}+\frac{k_2}{k_1}\right)}$$

$$= \frac{1}{\left(1+k_1\cdot\frac{1}{\sqrt{k_1k_2}}\right)\left(\frac{\sqrt{k_1k_2}}{k_1\cdot}+\frac{k_2}{k_1}\right)}$$

$$= \frac{1}{\left(1+\sqrt{\frac{k_1}{k_2}}\right)\left(\sqrt{\frac{k_2}{k_1}}+\frac{k_2}{k_1}\right)} = \frac{1}{\sqrt{\frac{k_2}{k_1}}+1+\frac{k_2}{k_1}+\sqrt{\frac{k_2}{k_1}}}$$

$$= \frac{1}{\frac{k_2}{k_1}+2\sqrt{\frac{k_2}{k_1}}+1}$$

$$\therefore\; \boxed{\frac{C_{R,max}}{C_{A0}} = \frac{1}{\left(\sqrt{\frac{k_2}{k_1}}+1\right)^2}}$$