

Immobilized Enzyme on a (CSTR) Reactor Surface with Product Inhibition (/w physical units followed by dimensionless analysis.)

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Operating parameters:

$F := 3 \cdot \text{cm}^3 \cdot \text{sec}^{-1}$... volumetric flow rate
$A := 100 \cdot \text{cm}^2$... surface area of immobilized enzyme
$s_f := 10 \cdot \text{gm} \cdot \text{liter}^{-1}$... feed substrate concentration
$k_L := 0.01 \cdot \text{cm} \cdot \text{sec}^{-1}$... mass transfer coefficient

Reaction rate parameters:

$v_m := 0.0001 \cdot \text{gm} \cdot \text{sec}^{-1} \cdot \text{cm}^{-2}$... maximum reaction rate
$K_m := 1 \cdot \text{gm} \cdot \text{liter}^{-1}$... Michaelis-Menten constant
$K_p := 1$... product inhibition constant

$$v(s, p) := \frac{v_m \cdot s}{K_m + s + K_p \cdot p}$$

Material balance equations for the rate of conversion are given below:

$$\begin{aligned} r_1(s_b) &:= F \cdot (s_f - s_b) \\ r_2(p_b) &:= F \cdot p_b \\ r_3(s_b, s) &:= A \cdot k_L \cdot (s_b - s) \\ r_4(p_b, p) &:= A \cdot k_L \cdot (p - p_b) \\ r_5(s, p) &:= A \cdot v(s, p) \end{aligned}$$

The above 5 equations can be reduced to the following equation:

$$\frac{F}{v_m \cdot A} \cdot \frac{s_f - s}{1 + \frac{F}{k_L \cdot A}} = \frac{s}{K_m + K_p \cdot s_f + (1 - K_p) \cdot s}$$

Non-dimensionalize the last equation with

$$\begin{aligned} x &:= \frac{s}{s_f} & K &:= \frac{K_m}{s_f} & \beta &:= \frac{F \cdot s_f}{v_m \cdot A} & \Gamma &:= \frac{F}{k_L \cdot A} & \alpha &:= \frac{\beta}{1 + \Gamma} \\ & & & & \beta &= 3 & \Gamma &= 3 & \alpha &= 0.75 \end{aligned}$$

Thus, the non-dimensional equation to be solved is:

$$f(x, \alpha, K, \Gamma) := \alpha \cdot (1 - x) - \frac{x}{K + K_p + (1 - K_p) \cdot x} = 0$$

Sample calculation based on the given parameters:

$$x := 1 \quad (\text{provide initial guess})$$

$$x := \text{root}(f(x, \alpha, K, K_p), x) \quad x = 0.452$$

$$s := x \cdot s_f \quad s = 4.521 \cdot \text{gm} \cdot \text{liter}^{-1} \quad \dots \text{Substrate conc. at the reaction surface}$$

$$p := s_f - s \quad p = 5.479 \cdot \text{gm} \cdot \text{liter}^{-1} \quad \dots \text{Product conc. at the reaction surface}$$

$$s_b := \frac{\Gamma \cdot s_f + s}{1 + \Gamma} \quad s_b = 8.63 \cdot \text{gm} \cdot \text{liter}^{-1} \quad \dots \text{Substrate conc. in the bulk phase or reactor exit}$$

$$p_b := \frac{p}{1 + \Gamma} \quad p_b = 1.37 \cdot \text{gm} \cdot \text{liter}^{-1} \quad \dots \text{Product conc. in the bulk phase or reactor exit}$$

Check (All rates should be identical):

$$r_1(s_b) = 0.00411 \cdot \text{gm} \cdot \text{sec}^{-1}$$

$$r_2(p_b) = 0.00411 \cdot \text{gm} \cdot \text{sec}^{-1}$$

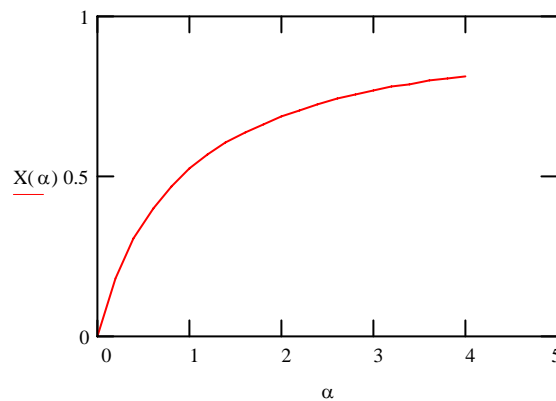
$$r_3(s_b, s) = 0.00411 \cdot \text{gm} \cdot \text{sec}^{-1}$$

$$r_4(p_b, p) = 0.00411 \cdot \text{gm} \cdot \text{sec}^{-1}$$

$$r_5(s, p) = 0.00411 \cdot \text{gm} \cdot \text{sec}^{-1}$$

Since α contains all the operating parameters, the effect of various operating conditions on conversion can be studied by varying α .

$$X(\alpha) := \text{root}(f(x, \alpha, K, K_p), x) \quad \alpha := 0, 0.2 \dots 4$$



α	$X(\alpha)$
0	0
0.2	0.18
0.4	0.306
0.6	0.398
0.8	0.468
1	0.524
1.2	0.569
1.4	0.606
1.6	0.638
1.8	0.664
2	0.687
2.2	0.708
2.4	0.725
2.6	0.741
2.8	0.755
3	0.767
3.2	0.779
3.4	0.789
3.6	0.798
3.8	0.807
4	0.814

3

4

0.815

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