

Immobilized Enzyme on a (CSTR) Reactor Surface with Product Inhibition --- Vary F, solve 1 eqn.
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Operating parameters:

$F := 0 \cdot \text{cm}^3 \cdot \text{sec}^{-1}, 0.5 \cdot \text{cm}^3 \cdot \text{sec}^{-1} .. 10 \cdot \text{cm}^3 \cdot \text{sec}^{-1}$... volumetric flow rate

$A := 100 \cdot \text{cm}^2$... surface area of immobilized enzyme

$s_f := 10 \cdot \text{g} \cdot \text{liter}^{-1}$... feed substrate concentration

$k_L := 0.01 \cdot \text{cm} \cdot \text{sec}^{-1}$... mass transfer coefficient

Reaction rate parameters:

$v_m := 0.0001 \cdot \text{g} \cdot \text{sec}^{-1} \cdot \text{cm}^{-2}$... maximum reaction rate

$K_m := 1 \cdot \text{g} \cdot \text{liter}^{-1}$... Michaelis-Menten constant

$K_p := 1$... product inhibition constant

Non-dimensionalized equations to be solved:

$$K := \frac{K_m}{s_f} \quad \beta(F) := \frac{F \cdot s_f}{v_m \cdot A} \quad \Gamma(F) := \frac{F}{k_L \cdot A} \quad \alpha(F) := \frac{\beta(F)}{1 + \Gamma(F)}$$

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

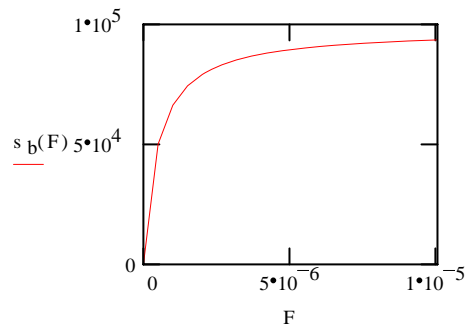
Solution:

$x := 1$... provide initial guess

$x(F) := \text{root}(f(x, F), x)$... find the solution

Substrate concentration in the bulk or reactor exit

$$s_b(F) := \frac{\Gamma(F) \cdot s_f + x(F) \cdot s_f}{1 + \Gamma(F)}$$



Rate of conversion (productivity)

$$r(F) := F \cdot (s_f - s_b(F))$$

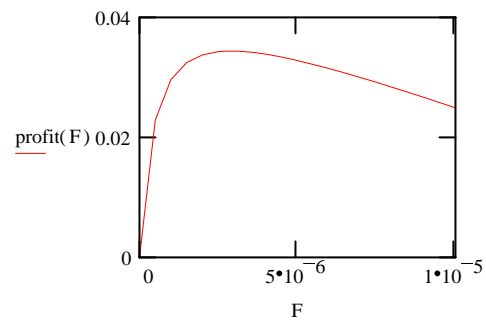


Profitability

relative_price := 0.02 ... (substrate price)/(product price)

material_cost(F) := relative_price · F · s_f

profit(F) := r(F) – material_cost(F)



In practice, there usually exists an optimal operating point where profit is maximized.