

Immobilized Enzyme on a (CSTR) Reactor Surface with Product Inhibition --- Vary both s_f & F , solve 1 eqn.

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Operating parameters:

$$\begin{aligned}
 i &:= 0..10 & F_i &:= 0 \cdot \text{cm}^3 \cdot \text{sec}^{-1} + i \cdot 0.5 \cdot \text{cm}^3 \cdot \text{sec}^{-1} & \dots & \text{volumetric flow rate} \\
 A &:= 100 \cdot \text{cm}^2 & & & \dots & \text{surface area of immobilized enzyme} \\
 j &:= 0..10 & s_{f_j} &:= 0.01 \cdot \text{g} \cdot \text{liter}^{-1} + j \cdot 10 \cdot \text{g} \cdot \text{liter}^{-1} & \dots & \text{feed substrate concentration} \\
 k_L &:= 0.01 \cdot \text{cm} \cdot \text{sec}^{-1} & & & \dots & \text{mass transfer coefficient}
 \end{aligned}$$

Reaction rate parameters:

$$\begin{aligned}
 v_m &:= 0.0001 \cdot \text{g} \cdot \text{sec}^{-1} \cdot \text{cm}^{-2} & \dots & \text{maximum reaction rate} \\
 K_m &:= 1 \cdot \text{g} \cdot \text{liter}^{-1} & \dots & \text{Michaelis-Menten constant} \\
 K_p &:= 1 & \dots & \text{product inhibition constant}
 \end{aligned}$$

Non-dimensionalized equations to be solved:

$$\begin{aligned}
 K(s_f) &:= \frac{K_m}{s_f} & \beta(F, s_f) &:= \frac{F \cdot s_f}{v_m \cdot A} & \Gamma(F) &:= \frac{F}{k_L \cdot A} & \alpha(F, s_f) &:= \frac{\beta(F, s_f)}{1 + \Gamma(F)} \\
 f(x, F, s_f) &:= \alpha(F, s_f) \cdot (1 - x) - \frac{x}{K(s_f) + K_p + (1 - K_p) \cdot x} = 0
 \end{aligned}$$

Solution:

$$\begin{aligned}
 x &:= 1 & \dots & \text{provide initial guess} \\
 x(F, s_f) &:= \text{root}(f(x, F, s_f), x) & \dots & \text{find the solution}
 \end{aligned}$$

Substrate concentration in the bulk or reactor exit

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

Rate of conversion (productivity)

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

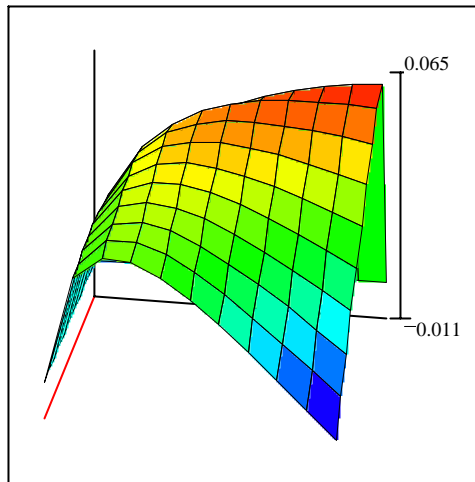
Profitability

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

material_cost(F, s_f) := relative_price · F · s_f

profit(F, s_f) := r(F, s_f) - material_cost(F, s_f)

profit_{i,j} := profit(F_i, s_{f,j})



profit

To maximize profit in this problem, one should use low F and high s_f ; however, the upper value of s_f in practice is limited by density or solubility of the substrate.