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

Instructor: Nam Sun Wang

Operating parameters:

$F := 3 \cdot cm^3 \cdot sec^{-1}$ ... volumetric flow rate

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

$s_f := 5 \cdot g \cdot liter^{-1}, 10 \cdot g \cdot liter^{-1} .. 100 \cdot g \cdot liter^{-1}$ ... feed substrate concentration

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

Reaction rate parameters:

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

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

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

Non-dimensionalized equations to be solved:

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

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

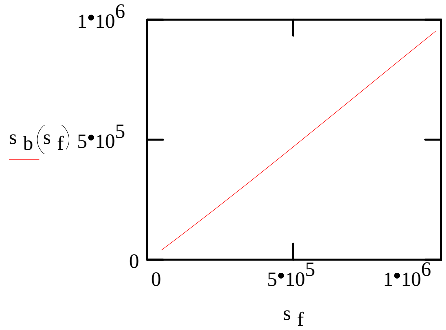
Solution:

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

$x(s_f) := root(f(x, s_f), x)$ ... find the solution

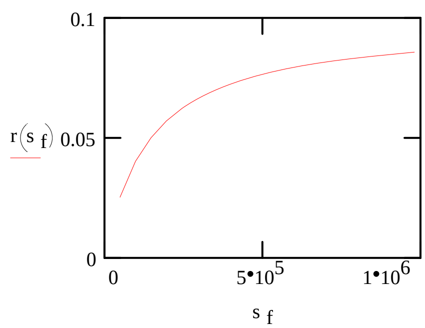
Substrate concentration in the bulk or reactor exit

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



Rate of conversion (productivity)

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

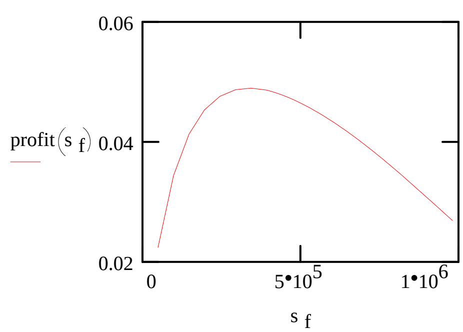


Profitability

$relative\_price := 0.02$ ... (substrate price)/(product price)

$material\_cost(s_f) := relative\_price \cdot F \cdot s_f$

$profit(s_f) := r(s_f) - material\_cost(s_f)$



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