Immobilized Enzyme on a (CSTR) Reactor Surface with Product Inhibition -- Vary both s_f & F, solve multiple equations symbolically.
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Operating parameters:

$F := 3$ ... volumetric flow rate (cm^3/sec)

$A := 100$ ... surface area of immobilized enzyme (cm^2)

$s_f := 0.01$ ... feed substrate concentration (g/cm^3)

$k_L := 0.01$ ... mass transfer coefficient (cm/sec)

Reaction rate parameters:

$v_m := 0.0001$ ... maximum reaction rate (g/sec-cm^2)

$K_m := 0.001$ ... Michaelis-Menten constant (g/cm^3)

$K_p := 1$ ... product inhibition constant (dimensionless)

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

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

Given

$r = F \cdot (s_f - s_b)$ ... substrate balance over the entire bioreactor

$r = F \cdot p_b$ ... product balance over the entire bioreactor

$r = A \cdot k_L \cdot (s_b - s)$ ...substrate balance on the reactive surface arising from diffusion

$r = A \cdot k_L \cdot (p - p_b)$ ... product balance on the reactive surface arising from diffusion

$r = A \cdot v(s,p)$ ... reaction rate on the reactive surface

The above 5 equations can be solved simultaneously and symbolically (turn on |Math|Smartmath| on the menu). Note that F and s_f are not provided prior to this point and an initial guess is not needed.

$$\mathrm{Find}(r, s_b, s, p_b, p) \rightarrow \begin{pmatrix} 10. \cdot F \cdot \dfrac{s_f}{(11. \cdot F + 1000. \cdot F \cdot s_f + 10.)} \\ F \cdot s_f \cdot \dfrac{(11. + 1000. \cdot s_f)}{(11. \cdot F + 1000. \cdot F \cdot s_f + 10.)} \\ s_f \cdot F \cdot \dfrac{(1. + 1000. \cdot s_f)}{(11. \cdot F + 1000. \cdot F \cdot s_f + 10.)} \\ 10. \cdot \dfrac{s_f}{(11. \cdot F + 1000. \cdot F \cdot s_f + 10.)} \\ s_f \cdot \dfrac{(10. \cdot F + 10.)}{(11. \cdot F + 1000. \cdot F \cdot s_f + 10.)} \end{pmatrix}$$

Copy the above formula into my own variable/function; however, these functions are not automatically updated when reaction parameters are changed. For example, when K_p=2, the analytical formula takes on a very different expression. The advantage is having the analytical expression. (Note that the 0th element is r, 1st element is s_b.)

$$rate(F, s_f) := 10.\cdot F\cdot\frac{s_f}{(11.\cdot F + 1000.\cdot F\cdot s_f + 10.)}$$

$$S_b(F, s_f) := F\cdot s_f\cdot\frac{(11. + 1000.\cdot s_f)}{(11.\cdot F + 1000.\cdot F\cdot s_f + 10.)}$$

Profitability

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

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

$profit(F, s_f) := rate(F, s_f) - material\_cost(F, s_f)$

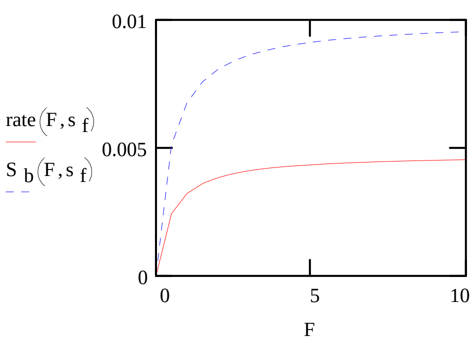
Solve for one operating point.

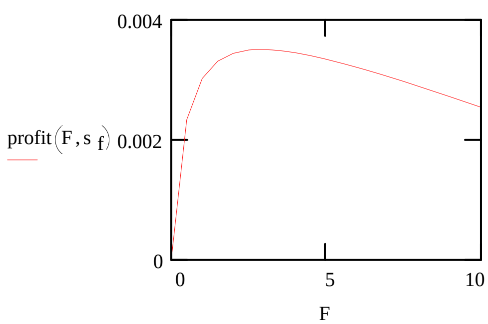
$F := 3$ $s_f := 0.01$

$rate(F, s_f) = 0.00411$ $profit(F, s_f) = 0.00351$

Vary flow rate

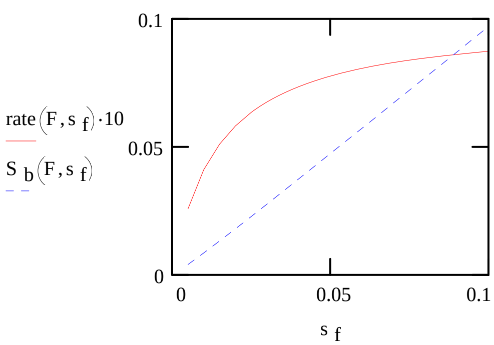
$F := 0, 0.5 .. 10$

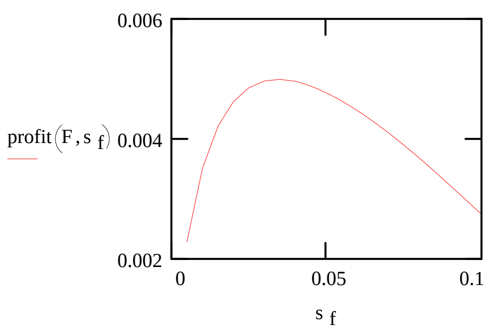




Vary substrate feed concentration

$F := 3$ $s_f := 0.005, 0.01 .. 0.1$





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

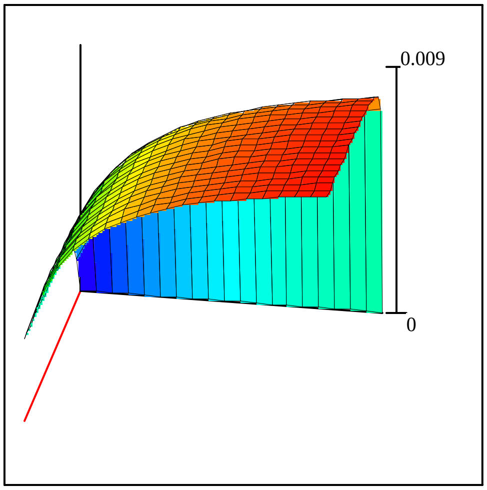
Vary both F and s_f. (Express results in a 2-D matrix that is more suitable for 3-D plotting)

$Ni := 20$ $\quad i := 0 .. Ni$ $\quad F_i := 0.5 \cdot i$

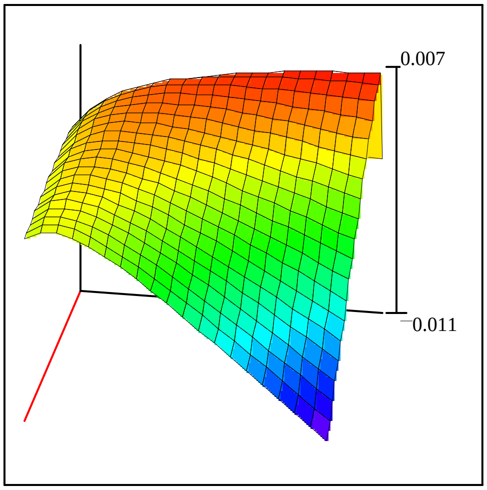
$Nj := 19$ $\quad j := 0 .. Nj$ $\quad s_{f_j} := 0.005 + 0.005 \cdot j$

$R_{i,j} := rate\left(F_i, s_{f_j}\right)$

$Profit_{i,j} := profit\left(F_i, s_{f_j}\right)$



R



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. (Note that high s_f is not necessarily good when there is substrate inhibition.)