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

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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:

$r := 0$ $s_b := 0$ $s := 0$ $p_b := 0$ $p := 0$ ...Initial guesses

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.

$\text{ans}(F, s_f) := \text{Find}(r, s_b, s, p_b, p)$

An example: $$\text{ans}(3, 0.01) = \begin{bmatrix} 0.004 \\ 0.009 \\ 0.005 \\ 0.001 \\ 0.005 \end{bmatrix}$$

Use my own variable names. (Note that the 0th element of ans is r, 1st element is s_b.)

$\text{rate}(F, s_f) := \text{ans}(F, s_f)_0$ $S_b(F, s_f) := \text{ans}(F, s_f)_1$

Profitability

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

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

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

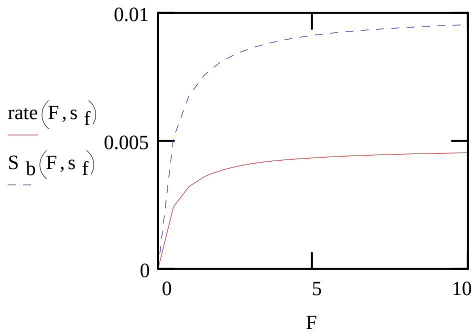
Solve for one operating point.

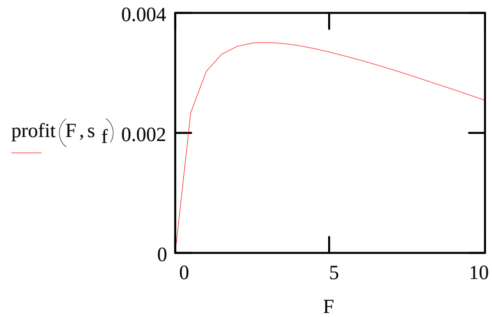
$F := 3$ $\qquad s_f := 0.01$

$\text{rate}(F, s_f) = 0.00411$ $\qquad \text{profit}(F, s_f) = 0.00351$

Vary flow rate

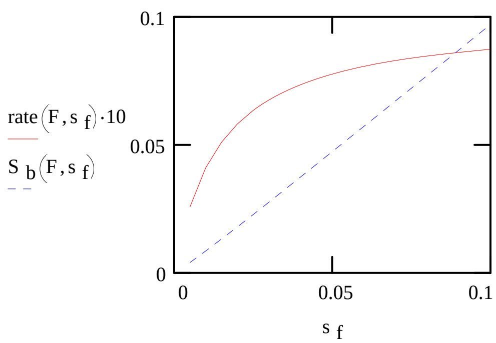
$F := 0, 0.5 .. 10$

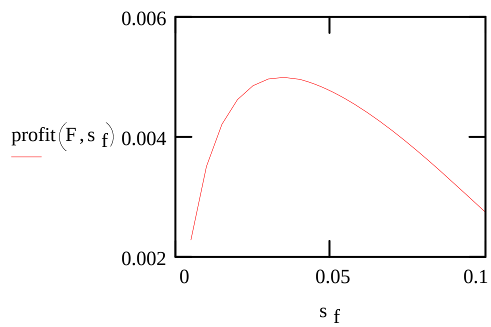




Vary substrate feed concentration

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





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

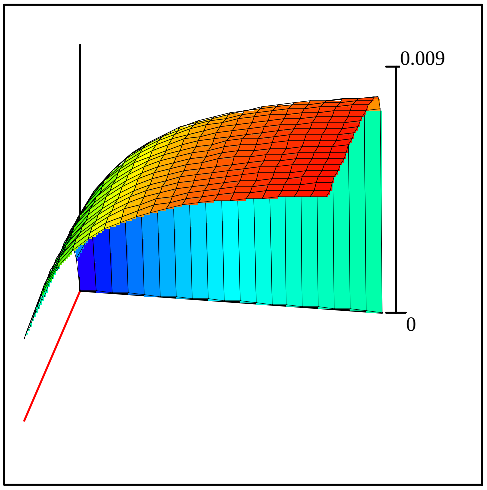
Vary both F and s_f. (Express results in a 2-D matrix that is more suitable for 3-D plotting)

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

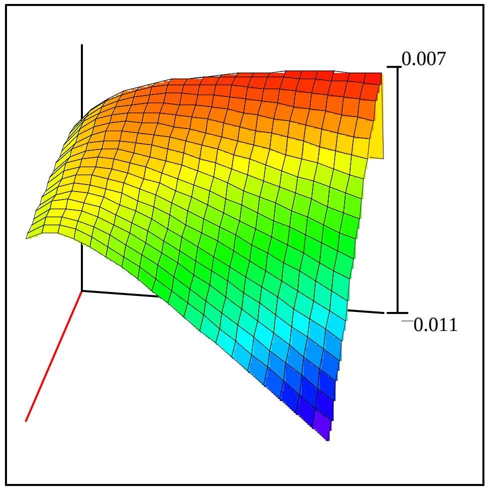
$Nj := 19 \qquad j := 0 .. Nj \qquad s_{f_j} := 0.005 + 0.005 \cdot j$

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

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



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.)

Range F and s_f instead of using subscripted indices, but tricky to convert into a matrix for plotting. (Note that the 0th element of ans is sb, 1st 20 solved for F=0, 2nd 20 solved for F=0.5, and so on.)

$F := 0, 0.5 .. 10 \qquad s_f := 0.005, 0.01 .. 0.1$

$S_b(F, s_f)$	$rate(F, s_f)$	$profit(F, s_f)$
0	0	0
0	0	0
0	0	0
0	0	0
0	0	0
0	0	0
0	0	0
0	0	0
0	0	0
0	0	0
0	0	0
0	0	0
0	0	0
0	0	0

0	0	0
0	0	0
0	0	0
0	0	0
0	0	0
0	0	0
0.002	0.001	0.001
0.005	0.002	0.002
0.008	0.003	0.003
0.012	0.004	0.004
0.016	0.004	0.004
0.02	0.005	0.005
0.024	0.005	0.005
0.029	0.006	0.005
0.033	0.006	0.005
0.038	0.006	0.006
0.042	0.006	0.006
0.047	0.007	0.006
0.051	0.007	0.006
0.056	0.007	0.006
0.061	0.007	0.006
0.066	0.007	0.006
0.07	0.007	0.006
0.075	0.007	0.007
0.08	0.008	0.007
0.085	0.008	0.007
0.003	0.002	0.002
0.007	0.003	0.003
0.011	0.004	0.004
0.015	0.005	0.004
0.02	0.005	0.005
0.024	0.006	0.005
0.029	0.006	0.006
0.033	0.007	0.006
0.038	0.007	0.006
0.043	0.007	0.006