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:

$$r_1(s_b, F, s_f) := F \cdot (s_f - s_b)$$
$$r_2(p_b, F) := F \cdot p_b$$
$$r_3(s_b, s) := A \cdot k_L \cdot (s_b - s)$$
$$r_4(p_b, p) := A \cdot k_L \cdot (p - p_b)$$
$$r_5(s,p) := A \cdot v(s,p)$$

The above 5 equations can be solved simultaneously.

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

Given

$$r_1(s_b, F, s_f) = r_2(p_b, F)$$
$$r_2(p_b, F) = r_3(s_b, s)$$
$$r_3(s_b, s) = r_4(p_b, p)$$
$$r_4(p_b, p) = r_5(s, p)$$
$$ans(F, s_f) := Find(s_b, s, p_b, p)$$

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

Rate of conversion (productivity). (Note that the 0th element of ans is s_b.)

$$r(F, s_f) := F \cdot \left(s_f - ans(F, s_f)_0\right)$$

Profitability

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

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

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

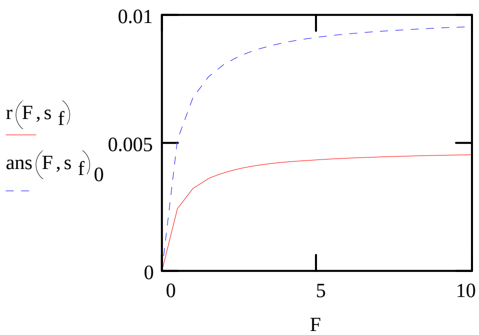
Solve for one operating point.

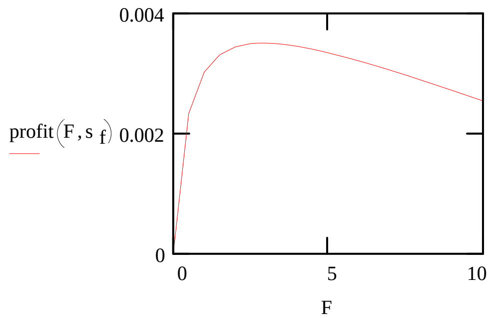
$F := 3 \qquad s_f := 0.01$

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

Vary flow rate

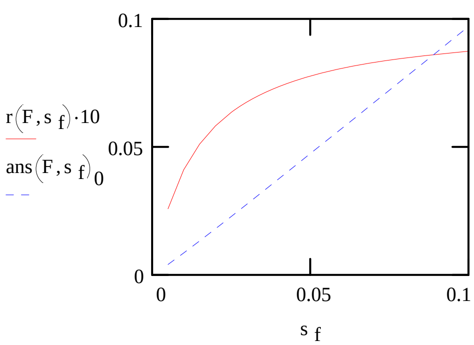
$F := 0, 0.5 .. 10$

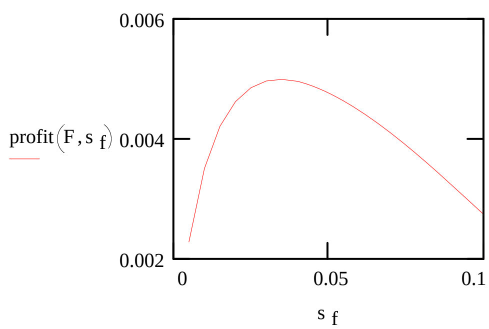




Vary substrate feed concentration

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





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

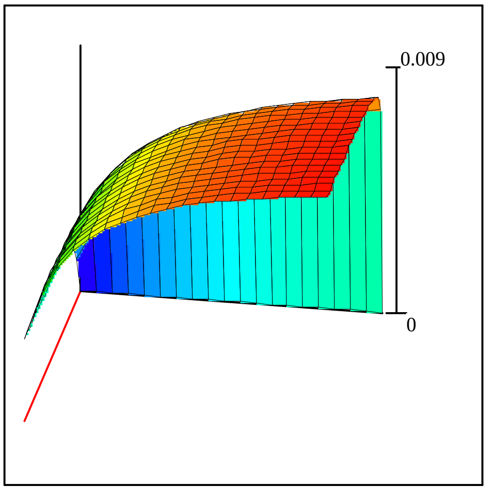
Vary both F and s_f. (Express results in a 2-D matrix that is more suitable for 3-D plotting)

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

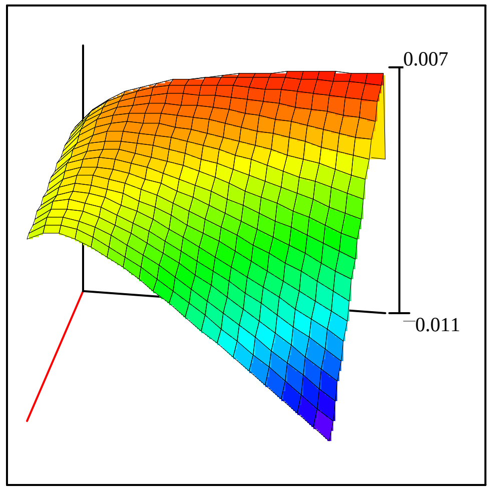
$Nj := 19$ $\quad j := 0 .. Nj$ $\quad s_{f_j} := 0.005 + 0.005 \cdot j$

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

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



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 s_b, 1st 20 solved for F=0, 2nd 20 solved for F=0.5, and so on.)

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

$ans\left(F, s_f\right)_0$	$r\left(F, s_f\right)$	$profit\left(F, s_f\right)$
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