

Heterogeneous catalysis with external mass transfer resistance (/w substrate inhibition).

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The substrate concentration at the reaction surface where enzyme is immobilized is determined by setting the rate of mass flux equal to the rate of reaction.

$k_1 := 0.0015$... mass transfer coefficient (cm/min)

$s_b := 0.02$... bulk substrate concentration (g/cm³)

Rate of mass flux: $J(s, s_b) := k_1 \cdot (s_b - s)$

$v_m := 0.0001$ (g/min-cm²)

$K_m := 0.001$ (g/cm³)

$K_i := 1000$ (cm³/g)

Rate of reaction:

$$v(s) := \frac{v_m \cdot s}{K_m + s + K_i \cdot s^2}$$

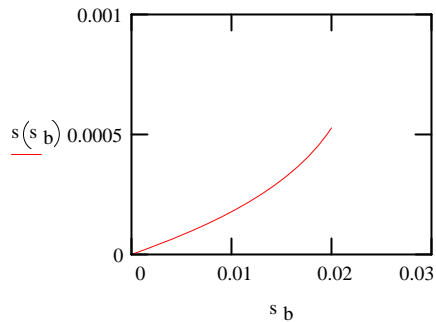
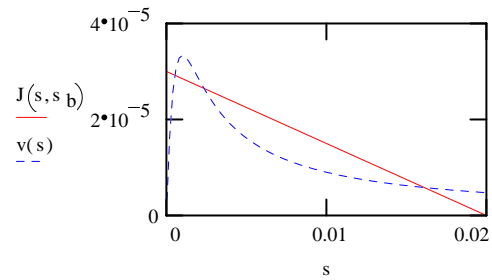
$s := 0, 0.01 \cdot s_b .. s_b$

Substrate concentration at surface

$s := 0$... initial guess

Note that other guesses may give different solutions

Given $J(s, s_b) = v(s)$ $s(s_b) := \text{Find}(s)$
 $s_b := 0, 0.001 .. 0.02$



Integrate the batch equation nstep := 100 i := 0 .. nstep t_f := 50 dt := $\frac{t_f}{nstep}$

A := 50000 ... Surface area (cm²):

V := 1000 ... Reactor volume (cm³):

$$ds_{b_i}/dt := -\frac{A \cdot k_1}{V} \cdot (s_{b_i} - s(s_{b_i})) \quad s_{b_0} := 0.02$$

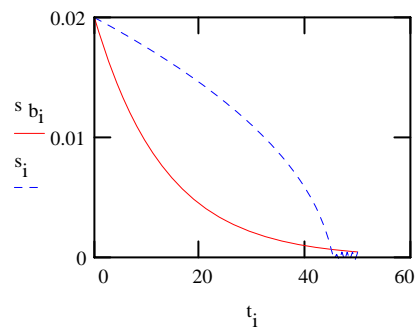
For some reason, "rkfixed" gets stuck when integration parameters are updated. Maybe MathCAD does not like my definition of the function s(s_b)

$$s_{b_{i+1}} := s_{b_i} + ds_{b_i}/dt \cdot dt \quad t_i := i \cdot dt$$

Integrate the batch equation without mass transfer limitation.

$$ds/dt := -\frac{A}{V} \cdot v(s) \quad s_0 := s_{b_0}$$

$$s_{i+1} := s_i + ds/dt(s_i) \cdot dt$$



Achieve a higher rate of conversion with mass transfer limitation!