Heterogeneous catalysis with external mass transfer resistance (/w substrate inhibition).
Damkohler Effectiveness Plot.
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The first equation characterizes mass transfer:

mass transfer coefficient: $k_l := 0.013$

bulk substrate concentration: $s_b := 20$

mass flux: $J(s) := k_l \cdot (s_b - s)$

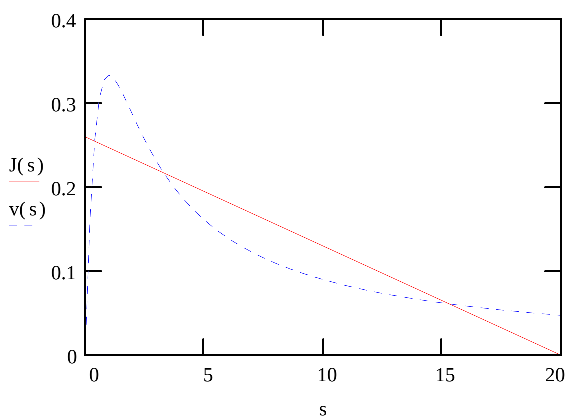
The second equation characterizes reaction:

rate constants: $v_m := 1$ $K_m := 1$ $K_i := 1$

rate of reaction: $v(s) := \dfrac{v_m \cdot s}{K_m + s + K_i \cdot s^2}$

At, steady state, the rate of substrate flux equals the rate of reaction (i.e., the intersection of two curves in the following plot).

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



The numerical solution is found with an initial guess of $s := 0$

$s := \mathrm{root}(J(s) - v(s), s)$

The substrate concentration at the reaction site (surface) is: $s = 0.395$

Effectiveness factor: $\eta = \dfrac{\text{actual\_rate}}{\text{rate\_without\_mass\_transfer\_resistance}}$ $\eta := \dfrac{v(s)}{v(s_b)}$

Thus, mass transfer resistance **increases** the rate of reaction by a factor of $\eta = 5.358$

The other two solutions can be obtained with different initial guesses of s.

Second solution: $s := 2.5$ $s := \mathrm{root}(J(s) - v(s), s)$ $s = 3.285$ $\eta := \dfrac{v(s)}{v(s_b)}$ $\eta = 4.587$

Third solution: $s := s_b$ $s := \mathrm{root}(J(s) - v(s), s)$ $s = 15.322$ $\eta := \dfrac{v(s)}{v(s_b)}$ $\eta = 1.285$

Generate Effectiveness Factor versus Damkohler plot by varying v_m.

Vary kinetic rate constant to achieve different Damkohler number.

$$i := 1 .. 1000 \qquad v_{m_i} := 0.1 \cdot i$$

Redefine v so that v_m is a parameter that can be varied.

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

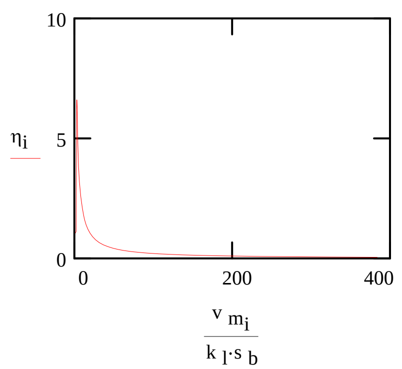
The numerical solution is found with an initial guess of $s := 0.1$

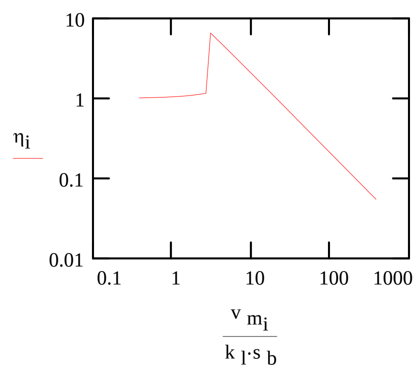
$$S_i := \mathrm{root}\left(J(s) - v\left(s, v_{m_i}\right), s\right)$$

The substrate concentration at the reaction site (surface) is S_i:

Effectiveness factor: $$\eta_i := \frac{v\left(S_i, v_{m_i}\right)}{v\left(s_b, v_{m_i}\right)}$$

Thus, mass transfer resistance reduces the rate of reaction by a factor of η.





The jump is due to a switch over from the lower solution to the upper solution.