

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: $k_1 := 1$

bulk substrate concentration: $s_b := 1$

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

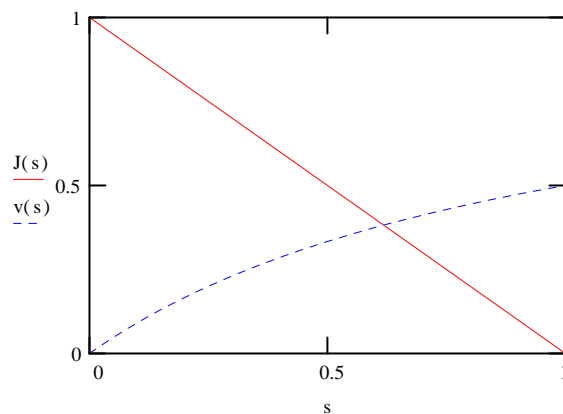
The second equation characterizes reaction:

rate constants: $v_m := 1 \quad K_m := 1 \quad K_i := 0$

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

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 $s := 0$

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

The substrate concentration at the reaction site (surface) is: $s = 0.618$

Effectiveness factor:
$$\eta = \frac{\text{actual_rate}}{\text{rate_without_mass_transfer_resistance}} \quad \eta := \frac{v(s)}{v(s_b)}$$

Thus, mass transfer resistance reduces the rate of reaction by a factor of $\eta = 0.764$

Generate Effectiveness Factor versus Damkohler plot by varying v_m .

Vary kinetic rate constant to achieve different Damkohler number.

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

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

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

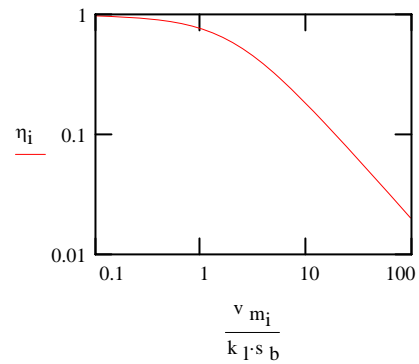
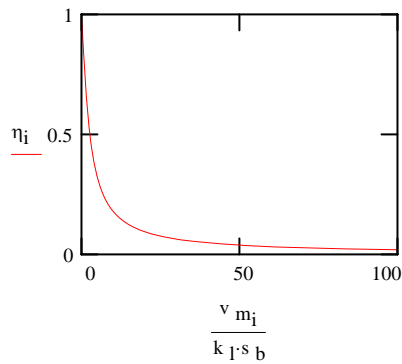
The numerical solution is found with an initial guess of $s := 0$

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

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

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

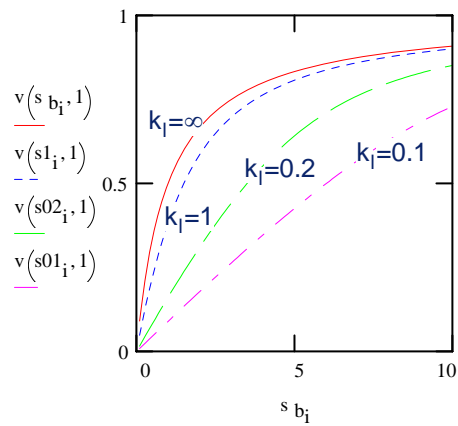
Thus, mass transfer resistance reduces the rate of reaction by a factor of η .



Apparent Reaction Rate. Vary substrate concentration and mass transfer coefficient to see how the observed reaction rate changes.

Redefine J so that s_b and k_l are parameters that can be varied. $J(s, s_b, k_l) := k_l \cdot (s_b - s)$

$$\begin{array}{llll}
 i := 1 .. 100 & s_{b_i} := 0.1 \cdot i & s1_i := \text{root}\left(J(s, s_{b_i}, 1) - v(s, 1), s\right) & k_l=1 \\
 & & s02_i := \text{root}\left(J(s, s_{b_i}, 0.2) - v(s, 1), s\right) & k_l=0.2 \\
 & & s01_i := \text{root}\left(J(s, s_{b_i}, 0.1) - v(s, 1), s\right) & k_l=0.1
 \end{array}$$



Mass transfer resistance increases the apparent value of K_m but does not affect the apparent value of v_m .