Find how the rate of conversion changes with the amount of enzyme immobilized in a spherical gel, or equivalently, v_m. Warning: It takes ~15 minutes to calculate/plot; be patient, or decrease the number of points of v_m in the plot.

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The following differential equation describes the substrate concentration in a spherical bead.

$$\frac{d^2 s}{dr^2} + \frac{2}{r}\cdot\frac{ds}{dr} = \frac{1}{D_e}\cdot v(s) \qquad \text{B.C.:} \quad s(R) = s_b \qquad \frac{ds(0)}{dr} = 0$$

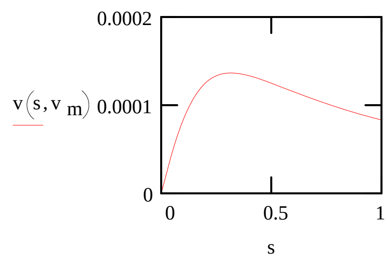
Assign model parameters and rate expression:

$v_m := 0.001$ g/L-sec $\qquad K_m := 1$ g/L $\qquad K_i := 10$ L/g

$D_e := 10^{-5}$ cm²/sec $\qquad R := 0.7$ cm $\qquad s_b := 1$ g/L

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

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



Transform the above equation into two 1st-order ODEs:

$dsdr(z) := z$

$$dzdr(r, s, z, v_m) := \frac{1}{D_e}\cdot v(s, v_m) - 2\cdot \text{if}\left(r = 0, \frac{1}{3\cdot D_e}\cdot v(s, v_m), \frac{z}{r}\right)$$

With $\quad ORIGIN := 1$

$$ODE(r, y) := \begin{bmatrix} dsdr(y_2) \\ dzdr(r, y_1, y_2, y_3) \\ 0 \end{bmatrix}$$

← Add a dummy ODE for $dv_m/dr=0$ so that we can vary v_m.

Integrate ODE to obtain s_R (the value of s at r=R) as we change s_0 (the value of s at r=0). $N := 100$

$$s_R(v_m, s_0) := \text{rkfixed}\left(\begin{bmatrix} s_0 \\ 0 \\ v_m \end{bmatrix}, 0, R, N, ODE\right)_{N,2}$$

The value of s at r=R depends on the value of s at r=0.

With the "Given-Find" function, numerically find the value of s_0 that yields $s(R)=s_R=s_b$

$s_0 := 0$ ... initial guess

Given $\quad s_R(v_m, s_0) = s_b \qquad s_0(v_m) := \text{Find}(s_0)$

An example: $s_0(v_m) = 0.08055$

Calculate the flux of substrate at the surface of bead by integrating the ODEs with the correct s_0 and taking the value of ds/dr at r=R.

$$dsdr_R(v_m) := \text{rkfixed}\left(\begin{bmatrix} s_0(v_m) \\ 0 \\ v_m \end{bmatrix}, 0, R, N, ODE\right)_{N,3}$$

Rate of conversion /w mass transfer resistance: $r(v_m) := 4\cdot\pi\cdot R^2\cdot D_e\cdot dsdr_R(v_m)$

Rate of conversion /wo mass transfer resistance: $r_{ideal}(v_m) := \frac{4}{3}\cdot\pi\cdot R^3\cdot v(s_b, v_m)$

Finally, we define the effectiveness factor.

$$\eta(v_m) := \frac{r(v_m)}{r_{ideal}(v_m)}$$

An example. $\eta(v_m) = 1.299$

Plot of reaction rate /w & /wo mass transfer resistance and effectiveness factor versus v_m. Note that both the reaction rates /w & /wo mass transfer resistance continue to increase with v_m, which is related to the enzyme level. However, the ratio of the two rates, which is the effectiveness factor, exhibits a maximum.

$v_m := 0.0002, 0.0004 .. 0.002$