Calculate the effectiveness factor η as a function of the Thiele modulus ϕ for an enzyme immobilized in a spherical gel. Warning: It takes ~15 minutes to calculate/plot η; be patient, or decrease the number of points of ϕ in the plot.

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

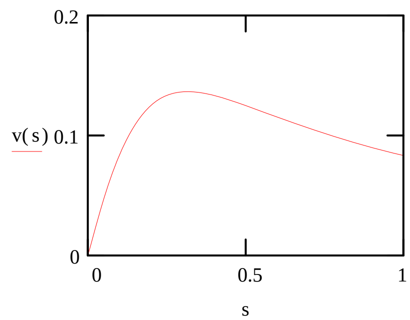
$$\frac{d^2 s}{dr^2} + \frac{2}{r}\cdot\frac{ds}{dr} = \phi^2\cdot v(s) \qquad \text{B.C.:} \quad s(1) = s_1 = 1 \qquad \frac{ds(0)}{dr} = 0$$

Assign dimensionless model parameters and rate expression:

$$\beta := 1 \qquad \Gamma := 10 \qquad \text{where} \qquad \beta = \frac{K_m}{s_b} \qquad \Gamma = K_i\cdot\frac{s_b}{\beta} \qquad \phi = R\cdot\sqrt{\frac{v_m}{D_e\cdot K_m}}$$

$$v(s) := \frac{s}{1 + \frac{s}{\beta} + \Gamma\cdot s^2}$$

$$s := 0, 0.01 .. 1$$



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

$$\mathrm{dsdr}(z) := z$$

$$\mathrm{dzdr}(r,s,z,\phi) := \phi^2\cdot v(s) - 2\cdot \mathrm{if}\left(r = 0, \frac{\phi^2}{3}\cdot v(s), \frac{z}{r}\right)$$

With $\mathrm{ORIGIN} := 1$

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

← Add a dummy ODE for $d\phi/dr=0$ so that we can vary ϕ.

Integrate ODE to obtain s_1 (the value of s at r=1) as we change s_0 (the value of s at r=0). $N := 100$

$$s_1(\phi, s_0) := \mathrm{rkfixed}\left(\begin{bmatrix} s_0 \\ 0 \\ \phi \end{bmatrix}, 0, 1, N, \mathrm{ODE}\right)_{N,2}$$

The value of s at r=1 is a function of the value of s at r=0.

With the "Given-Find" function, numerically find the value of s_0 that yields $s(1)=s_1=1$

$s_0 := 0$ ... initial guess

Given $\quad s_1(\phi, s_0) = 1 \qquad s_0(\phi) := \mathrm{Find}(s_0)$

An example: $s_0(7) = 0.08055$

Calculate 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=1.

$$\mathrm{dsdr}_1(\phi) := \mathrm{rkfixed}\left(\begin{bmatrix} s_0(\phi) \\ 0 \\ \phi \end{bmatrix}, 0, 1, N, \mathrm{ODE}\right)_{N,3}$$

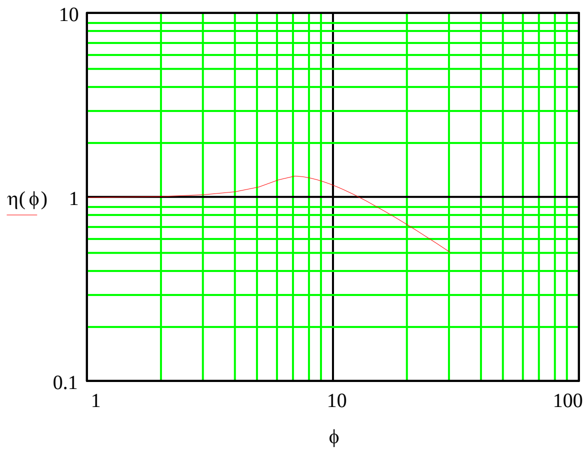
Finally, we define the effectiveness factor.

$$\eta(\phi) := \frac{dsdr_1(\phi)}{\frac{1}{3}\cdot\phi^2\cdot v(1)}$$

An example. $\eta(7) = 1.299$

Plot of Effectiveness factor versus Thiele modulus

$\phi := 1 .. 30$



There exists a maximum in the effectiveness factor where η is greater than unity. This is where mass transfer limitation allows the enzyme to face a lower level of substrate and shields the enzyme from the full inhibitory effect of substrate. To achieve the highest conversion rate, one can choose a bead radius to coincide with ϕ at the maximum η.

Side Bar: A Mathcad Trick. If we want to be able to change the initial guess, for example, to accommodate a wide range of ϕ so that the function s_0 converges quickly, we let the initial guess be part of the argument to the function s_0. Use this trick to provide different initial guesses to locate multiple roots.

Given $s_1(\phi, guess\_s_0) = 1$ $s_0(\phi, guess\_s_0) := Find(guess\_s_0)$

An example: $s_0(7, 0) = 0.08055$

Then, this argument propagates to the flux function $dsdr_1$.

$$dsdr_1(\phi, guess\_s_0) := rkfixed\left[\begin{bmatrix} s_0(\phi, guess\_s_0) \\ 0 \\ \phi \end{bmatrix}, 0, 1, N, ODE\right]_{N,3}$$

Finally, it propagates to the effectiveness factor η.

$$\eta(\phi, guess\_s_0) := \frac{dsdr_1(\phi, guess\_s_0)}{\frac{1}{3}\cdot\phi^2\cdot v(1)}$$

An example. $\eta(7, 0) = 1.299$