

Solve substrate concentration profile in a spherical gel (solution via the trial & error shooting method)  
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$$\frac{d^2 \cdot s}{dr^2} + \frac{2}{r} \cdot \frac{ds}{dr} = \phi^2 \cdot v(s) \quad \text{B.C.:} \quad s(1)=1 \quad \frac{ds(0)}{dr}=0$$

Dimensionless model parameters and rate expression:

$$\beta := 1 \quad \Gamma := 10$$

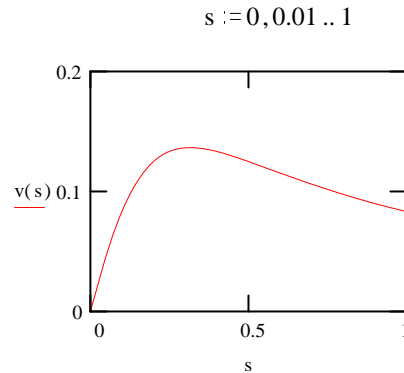
$$v(s) := \frac{s}{1 + \frac{s}{\beta} + \Gamma \cdot s^2}$$

$$\phi := 7$$

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

$$dsdr(r, s, z) := z$$

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



Provide/guess initial values

$$s_0 := 0.0805 \quad \leftarrow \text{unknown value (guess this value until } s_N=1)$$

$$z_0 := 0 \quad \leftarrow \text{known value}$$

Integrate ODE with the Euler's Method in  $N := 100$  steps, each step being  $dr := \frac{1}{N}$   $i := 0 \dots N$

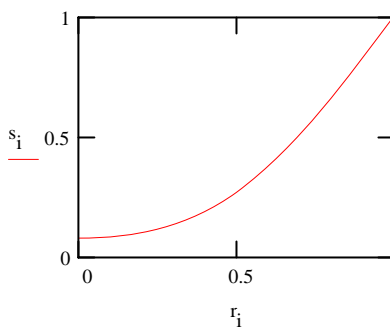
$$r_i := i \cdot dr \quad \dots \text{assign increments of } r$$

$$\begin{pmatrix} s_{i+1} \\ z_{i+1} \end{pmatrix} := \begin{pmatrix} s_i + dsdr(r_i, s_i, z_i) \cdot dr \\ z_i + dzdr(r_i, s_i, z_i) \cdot dr \end{pmatrix} \quad \dots \text{integrate } s \text{ and } z=ds/dr$$

Values at  $r=1$

$$s_N = 1.008 \quad z_N = 1.789$$

Plot of substrate profile



Compute the effectiveness factor, which is (observed rate / max rate without mass transfer limitation):

$$\eta := \frac{z_N}{\frac{1}{3} \cdot \phi^2 \cdot v(1)} \quad \eta = 1.314$$