Solve substrate/product concentration profiles in a spherical gel (WITH PRODUCT INHIBITION)
One two-point boundary value (TPBV) problem solved with "sbval"; will take 3 minutes.
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$$\frac{d^2 \cdot s}{dr^2} + \frac{2}{r} \cdot \frac{ds}{dr} = \phi^2 \cdot v(s) \qquad \text{B.C.:} \quad s(1) = 1 \qquad \frac{ds(0)}{dr} = 0$$

$$\frac{d^2 \cdot p}{dr^2} + \frac{2}{r} \cdot \frac{dp}{dr} = -\phi^2 \cdot v(s,p) \qquad \text{B.C.:} \quad p(1) = p1 \qquad \frac{dp(0)}{dr} = 0 \qquad \frac{dp(1)}{dr} = -\frac{ds(1)}{dr}$$

$p1 := 1$

(automatically true)

Dimensionless model parameters and rate expression:

$\beta := 1 \qquad \Gamma := 10 \qquad \gamma := 1$

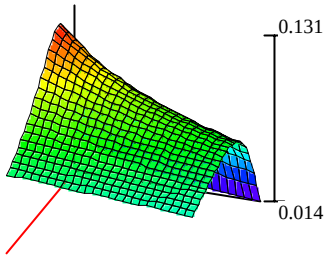
$$v(s,p) := \frac{s}{1 + \frac{s}{\beta} + \Gamma \cdot s^2 + \gamma \cdot p}$$

$\phi := 7$

$i := 1 .. 25 \quad s_i := i \cdot 0.05$

$j := 1 .. 25 \quad p_j := j \cdot 0.1$

$V_{i,j} := v(s_i, p_j)$



Transform the above equation into two 1st-order ODEs with the relationship: p=1+p1-s

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

$$dzdr(r,s,z) := \phi^2 \cdot v(s, 1 + p1 - s) - 2 \cdot \text{if}\left(r = 0, \frac{\phi^2}{3} \cdot v(s, 1 + p1 - s), \frac{z}{r}\right)$$

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

Use sbval function to evaluate the initial conditions:

$guess_1 := 0 \qquad y_{initial}(r, guess) := \begin{pmatrix} guess_1 \\ 0 \end{pmatrix} \qquad y_{final}(r,y) := y_1 - 1$ ← target is 1

$y0 := sbval(guess, 0, 1, ODE, y_{initial}, y_{final})$

$y0 = 0.295$ ← MathCAD's guess of s(0)

Set the initial condition:

$$y_{initial} := \begin{pmatrix} y0_1 \\ 0 \end{pmatrix}$$

Integrate ODE $N := 100 \quad i := 1 .. N$

$yout := rkfixed(y_{initial}, 0, 1, N, ODE)$

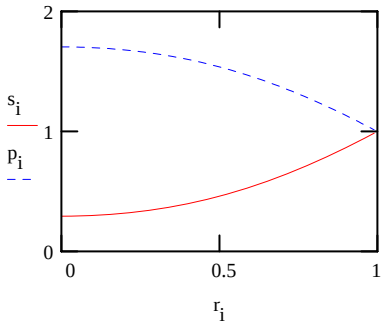
Use our own variable names

$r_i := yout_{i,1} \qquad s_i := yout_{i,2} \qquad dsdr_i := yout_{i,3}$

Values at r=1

$s_N = 0.986 \quad dsdr_N = 1.388$

Plot of substrate/product profiles $p_i := 1 + p1 - s_i$



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

$$\eta := \frac{dsdr_N}{\frac{1}{3}\cdot\phi^2\cdot v(1, p1)} \qquad \eta = 1.105$$