

Solve substrate/product concentration profiles in a spherical gel (WITH PRODUCT INHIBITION)  
 Two coupled two-point boundary value (TPBV) problems solved with "sbval"; will take 5-10 minutes.  
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$$\frac{d^2 \cdot s}{dr^2} + \frac{2}{r} \cdot \frac{ds}{dr} = \phi^2 \cdot v(s, p) \quad \text{B.C.:} \quad s(1) = 1 \quad \frac{ds(0)}{dr} = 0$$

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

$p1 := 1$  (automatically true)

Dimensionless model parameters and rate expression:

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

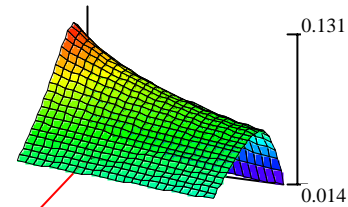
$$v(s, p) := \frac{s}{1 + \frac{s}{\beta} + \Gamma \cdot s^2 + \gamma \cdot p}$$

$$\phi := 7$$

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

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

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



Transform each of the above equations into two 1st-order ODEs for a total of four coupled ODEs:

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

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

$$dpdr(r, s, z, p, q) := q$$

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

$$\text{ODE}(r, y) := \begin{bmatrix} dsdr(r, y_1, y_2, y_3, y_4) \\ dzdr(r, y_1, y_2, y_3, y_4) \\ dpdr(r, y_1, y_2, y_3, y_4) \\ dqdr(r, y_1, y_2, y_3, y_4) \end{bmatrix}$$

Use sbval function to evaluate the initial conditions:

$$\text{guess} := \begin{pmatrix} 0 \\ 2 \end{pmatrix}$$

$$y_{\text{initial}}(r, \text{guess}) := \begin{bmatrix} \text{guess}_1 \\ 0 \\ \text{guess}_2 \\ 0 \end{bmatrix}$$

$$y_{\text{final}}(r, y) := \begin{pmatrix} y_1 - 1 \\ y_3 - p1 \end{pmatrix} \begin{matrix} \leftarrow \text{target is 1} \\ \leftarrow \text{target is p1} \end{matrix}$$

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

$$y0 = \begin{pmatrix} 0.295 \\ 1.705 \end{pmatrix} \begin{matrix} \leftarrow \text{MathCAD's guess of } s(0) \\ \leftarrow \text{MathCAD's guess of } p(0) \end{matrix}$$

Set the initial condition:

$$y_{\text{ initial}} := \begin{bmatrix} y0_1 \\ 0 \\ y0_2 \\ 0 \end{bmatrix}$$

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

$$y_{\text{out}} := \text{rkfixed}(y_{\text{ initial}}, 0, 1, N, \text{ODE})$$

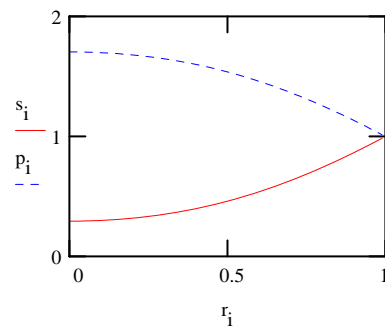
Use our own variable names

$$r_i := y_{\text{out}}_{i,1} \quad s_i := y_{\text{out}}_{i,2} \quad dsdr_i := y_{\text{out}}_{i,3} \quad p_i := y_{\text{out}}_{i,4} \quad dpdr_i := y_{\text{out}}_{i,5}$$

Values at  $r=1$

$$s_N = 0.986 \quad dsdr_N = 1.388 \quad p_N = 1.014 \quad dpdr_N = -1.388$$

Plot of substrate/product profiles in a bead



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

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