Solve substrate/product concentration profiles in a spherical gel (WITH PRODUCT INHIBITION)
Continuous bioreactor operated at steady-state. Note a major change in the B.C. at r=R.
One two-point boundary value (TPBV) problem solved with "sbval"; will take 3 minutes.
Instructor: Nam Sun Wang

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

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

(automatically true)

Model parameters:

$v_m := 0.00001$ g/cm^3-sec

$K_m := 0.001$ g/cm^3

$K_p := 1$

$$v(s,p) := \frac{v_m \cdot s}{K_m + s + K_p \cdot p}$$

$D_{es} := 10^{-5}$ cm^2/sec $\qquad D_{ep} := D_{es}$

Operating parameters:

$F := 100$ ... flow rate (cm^3/sec)

$s_f := 0.01$ ... substrate feed concentration (g/cm^3)

$V_b := 10000$ ... bead volume (cm^3)

$R := 0.7$ ... bead radius (cm)

$$A := \frac{3 \cdot V_b}{R}$$ ... total bead surface area (cm^2)

Continuous bioreactor operated at steady-state:

rate of diffusion across the bead surface = rate of conversion $\quad A \cdot D_{es} \cdot dsdr = F \cdot (s_f - s_b)$

stoichiometric conversion $\quad p_b = s_f - s_b$

Because of symmetry $\quad p = p_b + (s_b - s)$

Thus, the last two equations combine to give: $\quad p = s_f - s$

Transform the 2nd-order differential equation into two 1st-order ODEs with the relationship: $p=p_b+s_b-s$

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

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

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

Use sbval function to evaluate the initial conditions:

$guess_1 := 0$ $\quad y_{initial}(r, guess) := \begin{pmatrix} guess_1 \\ 0 \end{pmatrix}$ $\quad y_{final}(r, y) := A{\cdot}D_{es}{\cdot}y_2 - F{\cdot}(s_f - y_1)$

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

$y0 = 1.629 \cdot 10^{-4}$ ← MathCAD's guess of s(0), which is not refined enough for this problem.

Set the initial condition:

$y_{initial} := \begin{pmatrix} y0_1 \\ 0 \end{pmatrix}$ ... use sbval's value $\quad y_{initial} := \begin{pmatrix} 0.000163864 \\ 0 \end{pmatrix}$ ... guess manually

Integrate ODE $\quad N := 1000 \quad i := 1 .. N$

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

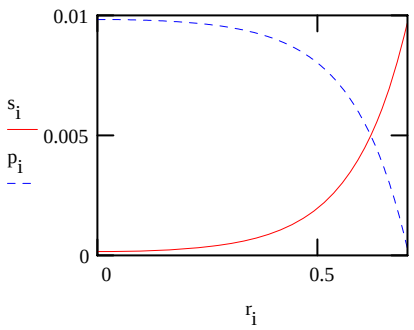
Use our own variable names

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

Values at r=1

$s_N = 0.00966$ $\quad dsdr_N = 0.0783$

Plot of substrate/product profiles $\quad p_i := s_f - s_i$



Check: (The next eqn. should be 0.)

$A{\cdot}D_{es}{\cdot}dsdr_N - F{\cdot}(s_f - s_N) = 1.59188 \cdot 10^{-6}$

Check: (The next 2 terms should be equal)

$F{\cdot}(s_f - s_N) = 0.03357$

$A{\cdot}D_{es}{\cdot}dsdr_N = 0.03357$

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

$\eta := \dfrac{A{\cdot}D_{es}{\cdot}dsdr_N}{V_b{\cdot}v(s_N, p_N)}$ $\quad \eta = 0.382$