Solve substrate concentration profile in a spherical gel with the "sbval" function.
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$$\frac{d^2 \cdot s}{dr^2} + \frac{2}{r} \cdot \frac{ds}{dr} = \phi^2 \cdot v(s) \qquad \text{B.C.:} \quad s(1) = 1 \qquad \frac{ds(0)}{dr} = 0$$

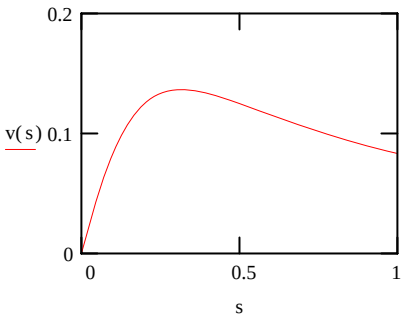
Dimensionless model parameters and rate expression:

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

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

$\phi := 7$

$s := 0, 0.01 .. 1$



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

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

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

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

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

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

$y0 = 0.074$

Set the initial condition:

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

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

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

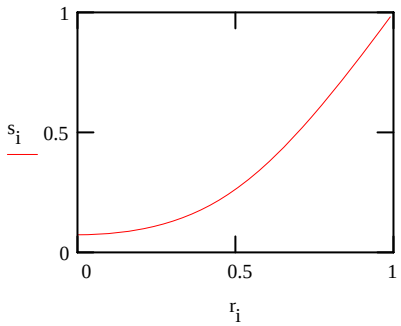
Use our own variable names

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

Values at r=1

$s_N = 0.982 \quad dsdr_N = 1.781$

Plot of substrate profile



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

$$\eta := \frac{dsdr_N}{\frac{1}{3}\cdot\phi^2\cdot v(1)} \qquad \eta = 1.309$$