Solve substrate concentration profile in a spherical gel (solution via "odesolve")
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Substrate diffusion in a spherical bead in the dimensionless form:

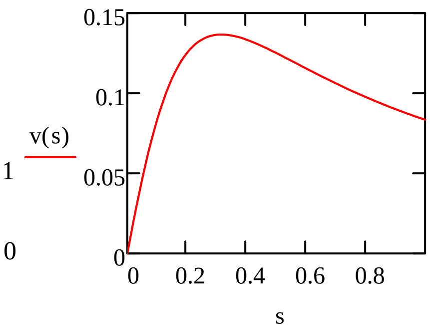
$$\frac{d^2 \cdot s}{dr^2} + \frac{2}{r} \cdot \frac{ds}{dr} = \varphi^2 \cdot v(s) \qquad \text{B.C.:} \quad s(1) = 1 \qquad \frac{ds(0)}{dr} = 0$$

Dimensionless model parameters and rate expression:

$$\beta := 1 \qquad \Gamma := 10 \qquad \varphi := 7$$

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

$$s := 0, 0.01 .. 1$$



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

Given

$$\frac{d}{dr}s(r) = z(r) \qquad \text{B.C.:} \quad s(1) = 1$$

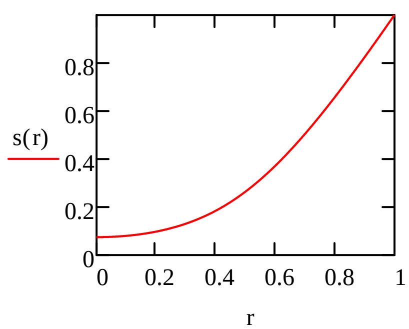
$$\frac{d}{dr}z(r) = \varphi^2 \cdot v(s(r)) - \text{if}\left(r = 0, \frac{2}{3} \cdot \varphi^2 \cdot v(s(r)), \frac{2}{r} \cdot z(r)\right) \qquad z(0) = 0$$

$$\begin{pmatrix} s \\ z \end{pmatrix} := \text{Odesolve}\left[\begin{pmatrix} s \\ z \end{pmatrix}, r, 1\right]$$

$$s(0) = 0.074 \qquad s(1) = 1$$

$$z(0) = 0 \qquad z(1) = 1.787$$

Plot of substrate profile



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

$$\eta := \frac{z(1)}{\frac{1}{3} \cdot \varphi^2 \cdot v(1)} \qquad \eta = 1.313$$

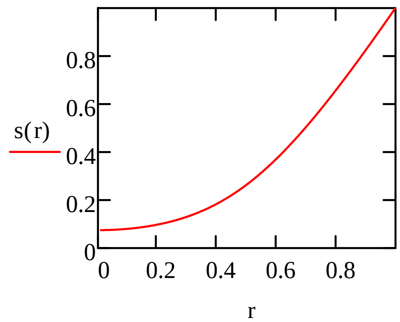
Another approach without decomposing into two 1st-order ODEs. The boundary condition must be in "prime" form, e.g, s'(0), which is entered with CTRL-F7. Furthermore, we need to extend the interval in "odesolve" to evaluate the derivative z(1) later. Since Mathcad considers the following to be only one equation, the "odesolve" function does not contain the argument "s".

Given

$$\frac{d^2}{dr^2}s(r) + \mathrm{if}\left[r = 0, \frac{2}{3}\cdot\varphi^2\cdot v(s(r)), \frac{2}{r}\cdot\left(\frac{d}{dr}s(r)\right)\right] = \varphi^2\cdot v(s(r))$$

B.C.: $s'(0) = 0$ $s(1) = 1$

$s := \mathrm{Odesolve}(r, 1.5)$



Double check B.C.

$s(0) = 0.074$ $s(1) = 1$

$z(r) := \frac{d}{dr}s(r)$ $z(1) = 1.787$

The following does not work because of 1/r at r=0

Given

$$\frac{d^2}{dr^2}s(r) + \frac{2}{r}\cdot\left(\frac{d}{dr}s(r)\right) = \varphi^2\cdot v(s(r))$$

B.C.: $s'(0) = 0$ $s(1) = 1$

$s := \mathrm{Odesolve}(r, 1.5)$

However, one can cheat without affecting numerical accuracy by starting at a value slightly above r=0.

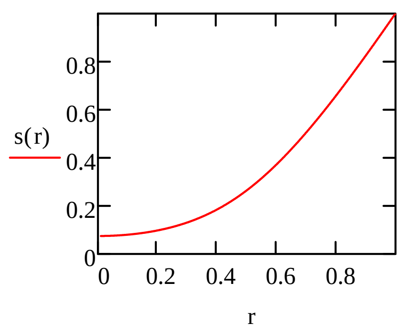
Given

$zero := 0.000000001$

$$\frac{d^2}{dr^2}s(r) + \frac{2}{r}\cdot\left(\frac{d}{dr}s(r)\right) = \varphi^2\cdot v(s(r))$$

B.C.: $s'(zero) = 0$ $s(1) = 1$

$s := \mathrm{Odesolve}(r, 1.5)$



Double check B.C.

$s(zero) = 0.074$ $s(1) = 1$

$z(r) := \frac{d}{dr}s(r)$ $z(1) = 1.787$