Solve substrate concentration profile in a spherical gel (solution via "odesolve", which presents a slightly different user interface over the same set of underlying engines such as "rkfixed" -- right click on "odesolve" to choose an underlying method. It is an interpolated version that gives a continuous function appearance.)

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Substrate diffusion in a spherical bead in the dimensionless form:

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

Dimensionless model parameters and rate expression:

\[
\beta := 1 \quad \Gamma := 10 \quad \varphi := 7 \quad v(s) := \frac{s}{1 + \frac{s}{\beta} + \Gamma \cdot s^2}
\]

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

Given

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

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

\[
\left( \begin{array}{c} s \\ z \end{array} \right) := \text{Odesolve} \left( \begin{array}{c} s \\ z \end{array} \right), r, 1
\]

The above BC can also be specified as "prime" with CTRL-F7, but not as \( \frac{d}{dr} \)

\[
\left( \begin{array}{c} s \\ z \end{array} \right) := \text{Odesolve} \left( \begin{array}{c} s \\ z \end{array} \right), r, 1
\]

Plot of substrate profile

Double check B.C.

\[
s(0) = 0.074 \quad s(1) = 1 \quad z(0) = 0 \quad z(1) = 1.787
\]

Compute the effectiveness factor, which is \( \frac{\text{observed rate}}{\text{max rate without mass transfer limitation}} \):

\[
\eta := \frac{z(1)}{\frac{1}{3} \cdot \varphi^2 \cdot v(1)} = 1.313 \quad \eta = 1.313
\]

Mathcad bug... The highest order derivative cannot appear more than once (i.e., \( \frac{dz}{dr} \) on RHS)

Given

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

\[
\frac{d}{dr} z(r) = \varphi^2 \cdot v(s(r)) - \text{if} \left( r = 0, \frac{2}{3} \cdot \varphi^2 \cdot v(s(r)), \frac{2}{r} \cdot z(r) \right) \quad z(0) = 0 \quad \left( \begin{array}{c} s \\ z \end{array} \right) := \text{Odesolve} \left( \begin{array}{c} s \\ z \end{array} \right), r, 1
\]
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 the "prime" under the tilde (~) key or CTRL-F7.

Furthermore, we need to extend the interval in "odesolve" to evaluate successfully the derivative \( z(1) \) later. Since Mathcad considers the following to be only one equation, the "odesolve" function does not contain the argument "s"; or include "s" entered as a 1x1 matrix.

Given

\[
\frac{d^2}{dr^2} s(r) + \left[ r = 0, \frac{2}{3} \varphi^2 \cdot v(s(r)), \frac{2}{r} \left( \frac{d}{dr} s(r) \right) \right] = \varphi^2 \cdot v(s(r)) \quad \text{B.C.: } s(0) = 0 \quad s(1) = 1
\]

\[s := \text{Odesolve}((s), r, 1.5)\]

Double check B.C.

\[s(0) = 0.074 \quad s(1) = 1\]

\[z(r) := \frac{d}{dr} s(r) \quad z(1) = 1.787\]

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

Given

\[
\frac{d^2}{dr^2} s(r) + \frac{2}{r} \left( \frac{d}{dr} s(r) \right) = \varphi^2 \cdot v(s(r)) \quad \text{B.C.: } s(0) = 0 \quad s(1) = 1
\]

\[s := \text{Odesolve}(r, 1)\]

However, one can cheat without affecting numerical accuracy by starting at a value slightly above \( r=0 \). Furthermore, the dependent variable (s in this case) need not be specified in Odesolve.

Given

\[\text{zero} := 0.000000001\]

\[
\frac{d^2}{dr^2} s(r) + \frac{2}{r} \left( \frac{d}{dr} s(r) \right) = \varphi^2 \cdot v(s(r)) \quad \text{B.C.: } s(\text{zero}) = 0 \quad s(1) = 1
\]

\[s := \text{Odesolve}(r, 1.5)\]

Double check B.C.

\[s(\text{zero}) = 0.074 \quad s(1) = 1\]

\[z(r) := \frac{d}{dr} s(r) \quad z(1) = 1.787\]
Prime notation in ODEs, as well as BCs

Given
\[ s''(r) + \frac{2}{r}(s'(r)) = \varphi^2 - v(s(r)) \]

B.C.: \[ s(\text{zero}) = 0 \quad s(1) = 1 \]

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

Double check B.C.
\[ s(\text{zero}) = 0.074 \quad s(1) = 1 \]
\[ z(r) := \frac{d}{dr}s(r) \quad z(1) = 1.787 \]

Parameterize (however NOT a truly parameterized function \( s(r, \varphi) \)).

Given
\[ s''(r) + \frac{2}{r}(s'(r)) = \varphi^2 - v(s(r)) \]

B.C.: \[ s(\text{zero}) = 0 \quad s(1) = 1 \]

\( s(\varphi) := \text{Odesolve}(r, 1.5) \quad s = f(\text{Unitless, Unitless}) \rightarrow \text{Unitless} \)

At this point \( s(\varphi) \) is a structure, not a function; it needs to be assigned to a function at a specific parameter value, for example, \( \varphi = 7 \) below.

\( \varphi = 7 \quad s := s(\varphi) \)

Double check B.C.
\[ s(\text{zero}) = 0.074 \quad s(1) = 1 \]
\[ z(r) := \frac{d}{dr}s(r) \quad z(1) = 1.787 \]