ENCH482 In-class demo on how to solve ODEs with Mathcad
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Dynamic simulation of enzyme kinetics

(Comparison of elementary mass action with the Michaelis-Menten expression)

$k_1 := 10$ $k_2 := 1$

E + S <----------> ES ----------> E + P (Reaction rate constants are specified.)

$k_i := 10$

Specify the ODEs.

$E_0 := 1$ $S_0 := 1$

Given

$\frac{d}{dt}E(t) = -k_1 \cdot E(t) \cdot S(t) + k_i \cdot ES(t) + k_2 \cdot ES(t)$ I.C.: $E(0) = E_0$ ...enzyme

$\frac{d}{dt}S(t) = -k_1 \cdot E(t) \cdot S(t) + k_i \cdot ES(t)$ $S(0) = S_0$ ...substrate

$\frac{d}{dt}ES(t) = k_1 \cdot E(t) \cdot S(t) - k_i \cdot ES(t) - k_2 \cdot ES(t)$ $ES(0) = 0$ ...enzyme-substrate complex

$\frac{d}{dt}P(t) = k_2 \cdot ES(t)$ $P(0) = 0$ ...product

$\begin{pmatrix} E \\ S \\ ES \\ P \end{pmatrix} := \text{odesolve}\left[\begin{pmatrix} E \\ S \\ ES \\ P \end{pmatrix}, t, 5\right]$

The default number of steps is 1000.
The solutions are 4 separate functions of t; E(t),S(t), ES(t), & P(t

Michaelis-Menten rate constants

$\mu_{max} := k_2 \cdot E_0$ $K_m := \frac{k_i + k_2}{k_1}$

Michaelis-Menten rate expression

Given

$\frac{d}{dt}s(t) = \frac{-\mu_{max} \cdot s(t)}{K_m + s(t)}$ $s(0) = S_0$

$S_{mm} := \text{odesolve}(t, 5)$ Do not specify dependent variable in "odesolve" when there is only one.

Plot of various concentrations

Simulation Parameters: $k_1 = 10$ $k_i = 10$ $k_2 = 1$ $E_0 = 1$ $S_0 = 1$