ENCH482 In-class demo on how to solve ODEs with MathCAD (with the Euler's Method)
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Dynamic simulation of enzyme kinetics

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

$k_1 := 1 \qquad k_2 := 10$

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

$k_i := 1$

Specify the ODEs.

$dEdt(t, E, S, ES, P) := -k_1 \cdot E \cdot S + k_i \cdot ES + k_2 \cdot ES$ ...dE/dt ...enzyme

$dSdt(t, E, S, ES, P) := -k_1 \cdot E \cdot S + k_i \cdot ES$ ...dS/dt ...substrate

$dESdt(t, E, S, ES, P) := k_1 \cdot E \cdot S - k_i \cdot ES - k_2 \cdot ES$ ...dES/dt ...enzyme-substrate complex

$dPdt(t, E, S, ES, P) := k_2 \cdot ES$ ...dP/dt ...product

Initial Conditions: $E_0 := 0.1 \qquad S_0 := 1 \qquad ES_0 := 0. \qquad P_0 := 0.$

Solve coupled set of ODEs with the Euler's Method.

(solve from $t_0 := 0$ to $t_f := 10$ in $nstep := 1000$ steps, with a step size of $h := \frac{t_f}{nstep}$

$i := 0 .. nstep$

(Note: coupled equations must be grouped together in a vector.)

$$\begin{bmatrix} t_{i+1} \\ E_{i+1} \\ S_{i+1} \\ ES_{i+1} \\ P_{i+1} \end{bmatrix} := \begin{bmatrix} h \cdot i \\ E_i + dEdt(t_i, E_i, S_i, ES_i, P_i) \cdot h \\ S_i + dSdt(t_i, E_i, S_i, ES_i, P_i) \cdot h \\ ES_i + dESdt(t_i, E_i, S_i, ES_i, P_i) \cdot h \\ P_i + dPdt(t_i, E_i, S_i, ES_i, P_i) \cdot h \end{bmatrix}$$

Michaelis-Menten rate constants

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

Michaelis-Menten rate expression

$sdot(s) := \frac{-\mu_{max} \cdot s}{K_m + s} \qquad S_{mm_0} := S_0$

$S_{mm_{i+1}} := S_{mm_i} + sdot(S_{mm_i}) \cdot h$

Plot of various concentrations $i := 1 .. nstep$