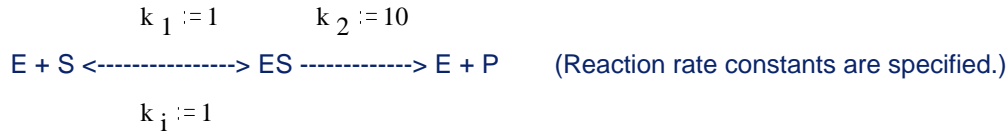


ENCH482 In-class demo on how to solve ODEs with MathCAD (with the Euler's Method)
 Instructor: Nam Sun Wang

Dynamic simulation of enzyme kinetics

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



Specify the ODEs.

$$\begin{array}{l}
 dEdt(t, E, S, ES, P) := -k_1 \cdot E \cdot S + k_1 \cdot ES + k_2 \cdot ES \quad \dots dE/dt \quad \dots \text{enzyme} \\
 dSdt(t, E, S, ES, P) := -k_1 \cdot E \cdot S + k_1 \cdot ES \quad \dots dS/dt \quad \dots \text{substrate} \\
 dESdt(t, E, S, ES, P) := k_1 \cdot E \cdot S - k_1 \cdot ES - k_2 \cdot ES \quad \dots dES/dt \quad \dots \text{enzyme-substrate complex} \\
 dPdt(t, E, S, ES, P) := k_2 \cdot ES \quad \dots dP/dt \quad \dots \text{product}
 \end{array}$$

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

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

$$\begin{array}{l}
 (\text{solve from } t_0 := 0 \quad \text{to } t_f := 10 \quad \text{in } nstep := 1000 \quad \text{steps, with a step size of } h := \frac{t_f}{nstep} \\
 i := 0 \dots nstep
 \end{array}$$

(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

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

Michaelis-Menten rate expression

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

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

Plot of various concentrations $i := 1 \dots nstep$

