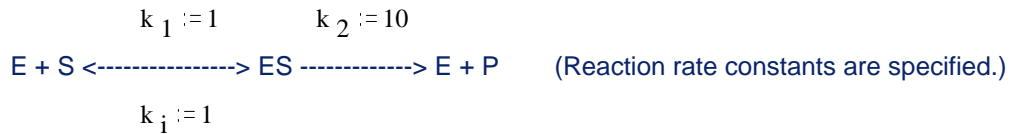


ENCH482 In-class demo on how to solve ODEs with MathCAD
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Dynamic simulation of enzyme kinetics

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



Specify the ODE as a vector equation. (Since MathCAD's index starts from 0, set ORIGIN=1)

$$\text{ydot}(t, y) := \begin{bmatrix} -k_1 \cdot y_1 \cdot y_2 + k_i \cdot y_3 + k_2 \cdot y_3 \\ -k_1 \cdot y_1 \cdot y_2 + k_i \cdot y_3 \\ k_1 \cdot y_1 \cdot y_2 - k_i \cdot y_3 - k_2 \cdot y_3 \\ k_2 \cdot y_3 \end{bmatrix} \begin{array}{l} \dots dE/dt \dots \text{enzyme} \\ \dots dS/dt \dots \text{substrate} \\ \dots dES/dt \dots \text{enzyme-substrate complex} \\ \dots dP/dt \dots \text{product} \end{array}$$

Initial Conditions: $E_0 := 0.1$ $S_0 := 1$

$$y_{\text{initial}} := \begin{bmatrix} E_0 \\ S_0 \\ 0 \\ 0 \end{bmatrix} \begin{array}{l} \dots E \\ \dots S \\ \dots ES \\ \dots P \end{array}$$

Solve coupled set of ODEs (solve from $t_0 := 0$ to $t_f := 10$ in $nstep := 100$ $i := 1 \dots nstep$)

$$\text{yout} := \text{rkfixed}(y_{\text{initial}}, t_0, t_f, nstep, \text{ydot})$$

$$t := \text{yout}^{\langle 1 \rangle} \quad E := \text{yout}^{\langle 2 \rangle} \quad S := \text{yout}^{\langle 3 \rangle} \quad ES := \text{yout}^{\langle 4 \rangle} \quad P := \text{yout}^{\langle 5 \rangle}$$

Michaelis-Menten rate constants

$$v_{\text{max}} := k_2 \cdot E_0 \quad K_m := \frac{k_i + k_2}{k_1}$$

Michaelis-Menten rate expression (Needed to add a dummy equation to solve)

$$\text{sdot}(t, s) := \frac{-v_{\text{max}} \cdot s_1}{K_m + s_1} \quad s_{\text{initial}_1} := S_0$$

$$\text{sout} := \text{rkfixed}(s_{\text{initial}_1}, t_0, t_f, nstep, \text{sdot})$$

$$S_{\text{mm}} := \text{sout}^{\langle 2 \rangle}$$

Comparison of Elementary Mass Action and Michaelis-Menten Kinetics

Elementary Mass Action Constants: $k_1 = 1$ $k_i = 1$ $k_2 = 10$

Michaelis-Menten Kinetic Constants: $v_{\max} = 1$ $K_m = 11$

Initial Concentrations: $S_0 = 1$ $E_0 = 0.1$

Plot of various concentrations

