ENCH482 In-class demo on how to solve ODEs with MathCAD
Instructor: Nam Sun Wang

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

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

$$ydot(t,y) := \begin{bmatrix} dEdt(t,y_1,y_2,y_3,y_4) \\ dSdt(t,y_1,y_2,y_3,y_4) \\ dESdt(t,y_1,y_2,y_3,y_4) \\ dPdt(t,y_1,y_2,y_3,y_4) \end{bmatrix}$$

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

$$y_{initial} := \begin{bmatrix} E_0 \\ S_0 \\ 0 \\ 0 \end{bmatrix} \begin{matrix} \text{...E} \\ \text{...S} \\ \text{...ES} \\ \text{...P} \end{matrix}$$

Solve coupled set of ODEs (solve from $t_0 := 0$ to $t_f := 5$ in $nstep := 1000$

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

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

Michaelis-Menten rate constants

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

Michaelis-Menten rate expression

$sdot(t,s) := \dfrac{-\mu_{max} \cdot s_1}{K_m + s_1}$ $s_{initial_1} := S_0$

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

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

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

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