

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

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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)

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

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

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

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

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

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

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

Michaelis-Menten rate constants

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

Michaelis-Menten rate expression

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

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

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

### 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

