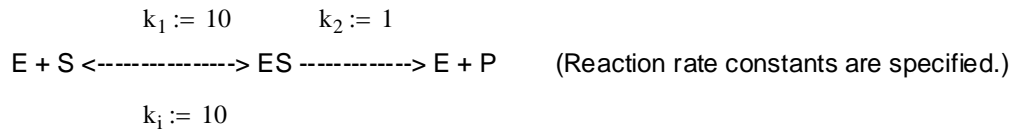


ENCH482 In-class demo on how to solve ODEs with Mathcad  
Instructor: Nam Sun Wang

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Dynamic simulation of enzyme kinetics

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



Specify the ODEs.

$$E_0 := 1 \quad S_0 := 1$$

Given

$$\begin{array}{ll}
 \frac{d}{dt} E(t) = -k_1 \cdot E(t) \cdot S(t) + k_i \cdot ES(t) + k_2 \cdot ES(t) & \text{I.C.: } E(0) = E_0 \quad \dots \text{enzyme} \\
 \frac{d}{dt} S(t) = -k_1 \cdot E(t) \cdot S(t) + k_i \cdot ES(t) & S(0) = S_0 \quad \dots \text{substrate} \\
 \frac{d}{dt} ES(t) = k_1 \cdot E(t) \cdot S(t) - k_i \cdot ES(t) - k_2 \cdot ES(t) & ES(0) = 0 \quad \dots \text{enzyme-substrate complex} \\
 \frac{d}{dt} P(t) = k_2 \cdot ES(t) & P(0) = 0 \quad \dots \text{product}
 \end{array}$$

$$\begin{pmatrix} E \\ S \\ ES \\ P \end{pmatrix} := \text{odesolve} \left[ \begin{pmatrix} E \\ S \\ ES \\ P \end{pmatrix}, t, 5 \right]$$

The default number of steps is 1000.  
The solutions are 4 separate functions of t; E(t), S(t), ES(t), & P(t)

Michaelis-Menten rate constants

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

Michaelis-Menten rate expression

Given

$$\frac{d}{dt} s(t) = \frac{-\mu_{\max} \cdot s(t)}{K_m + s(t)} \quad s(0) = S_0$$

$$S_{\text{mm}} := \text{odesolve}(t, 5) \quad \text{Do not specify dependent variable in "odesolve" when there is only one.}$$

Plot of various concentrations

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

