

# 1 Rate of Changes

Assume:

- At the beginning of the reaction, the amount of products produced is so small that the inverse reaction can be disregarded.
- The substrate concentration is much larger than that of the free enzyme, so that the substrate concentration remains essentially constant during the reaction.
- The second step of the reaction is the rate-limiting step of the reaction to ensure that the rate of ES decomposition to P is not sufficient to disrupt the equilibrium between E and ES.

Define the concentrations of the reactants as  $[E]$ ,  $[ES]$ ,  $[P]$ ,  $[S]$  the rate of change of reactants with time t:

$$V_E = \frac{d[E]}{dt} = -k_1[E][S] + k_2[ES] + k_3[ES]$$

$$V_S = \frac{d[S]}{dt} = -k_1[E][S] + k_2[ES]$$

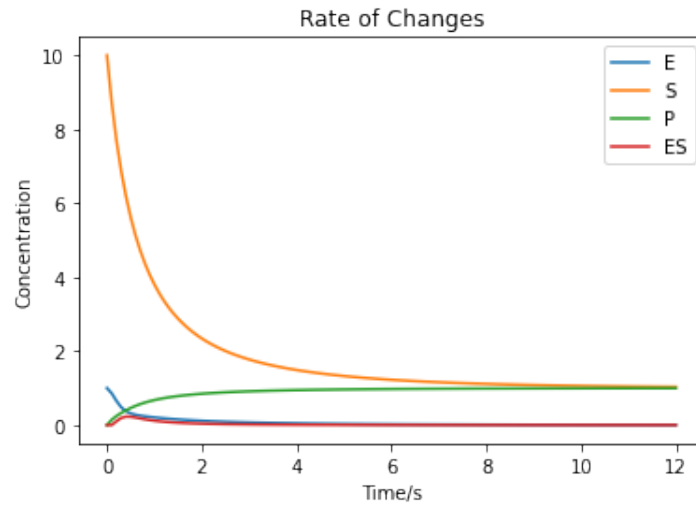
$$V_{ES} = \frac{d[ES]}{dt} = k_1[E][S] - k_2[ES] - k_3[ES]$$

$$V_P = \frac{d[P]}{dt} = k_3[ES]$$

## 2 Fourth-order Runge-Kutta

**Given:**  $k_1 = 100 \mu\text{M}/\text{min}$ ,  $k_2 = 600 \mu\text{M}/\text{min}$ ,  $k_3 = 150 \mu\text{M}/\text{min}$ ;  $E = 1.0 \mu\text{M}$ ;  $S = 10 \mu\text{M}$ ;

The rate of changes are plotted as below:



## 3 Velocity

The velocity  $V$  as a function of the concentration of the substrate  $S$  is defined by the Michaelis-Menten equation:

$$V = \frac{V_{max}[S]}{K_M + [S]}$$

The function is plotted as follows: The maximum velocity is 72.1724322962807

