Q 2

1. Defining the concentrations of P, S, ES and E are [P], [S], [ES] and [E], the rate of changes of the four species:

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

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

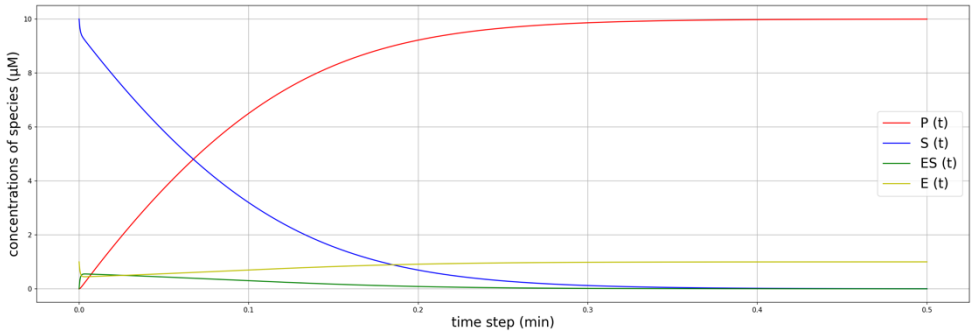
$$\frac{d[ES]}{dt} = k_1 \cdot [E] \cdot [S] - (k_2 + k_3) \cdot [ES]$$

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

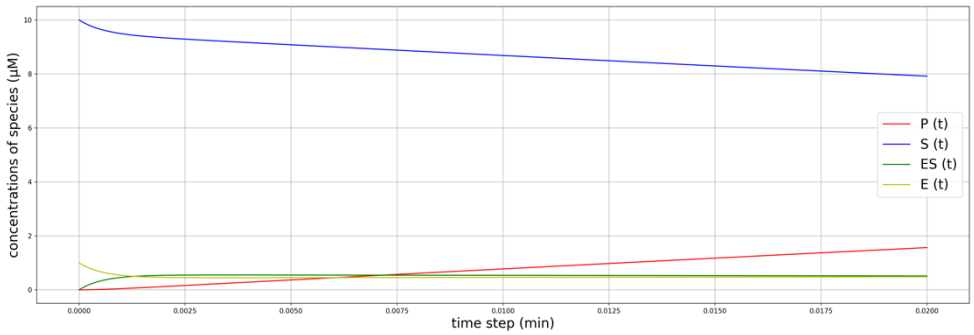
2. Code is presented in the github Q2 folder.

   Starting with the condition given: “initial concentration of E is 1 µM, the initial concentration of S is 10 µM, and the initial concentrations of ES and P are both 0”

   The simulated concentrations of P, S, ES and E are generated by the fourth-order Runge-Kutta method with start time 0.0 min, end time 0.5 min and 100000 steps, h = 0.000005 min/step.



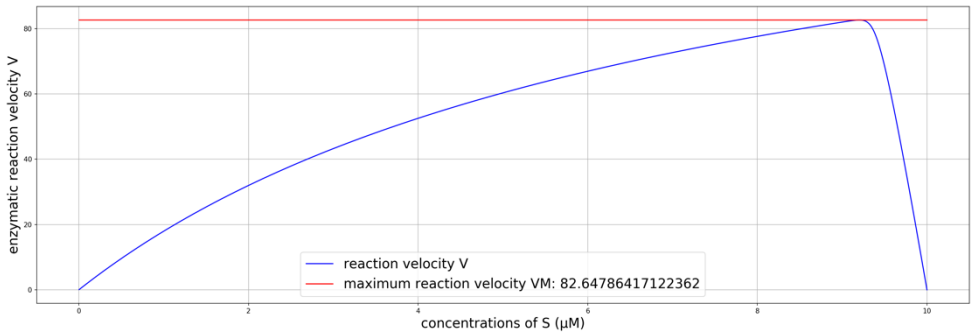
   To be precise, with start time 0.0 min, end time 0.02 min and 100000 steps, h = 0.0000002 min/step, the simulated concentrations of P, S, ES and E are generated to simulate the beginning stage when the concentration of substrate S is high.



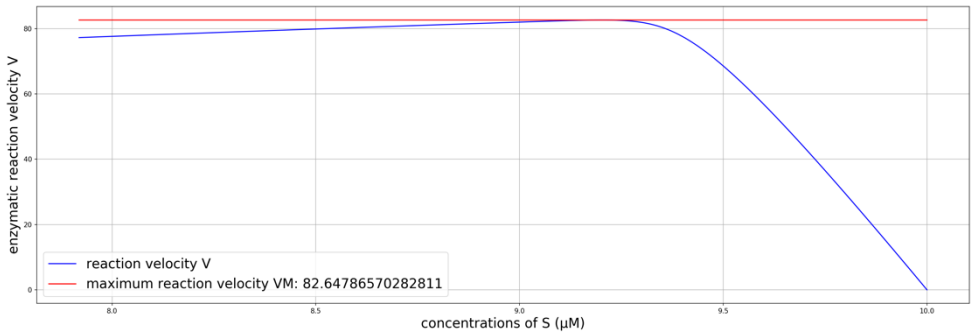
3. Code is presented in the github Q2 folder.

   Because of the velocity $V = \frac{d[P]}{dt} = k_3 \cdot [ES]$, the V-S plot can be viewed as follows:

   1. with start time 0.0 min, end time 0.5 min and 100000 steps, h = 0.000005 min/step.



   2. with start time 0.0 min, end time 0.02 min and 100000 steps, h = 0.0000002 min/step.



Reference:

1. Mass Action :

https://www.youtube.com/watch?v=eDMd4SAY7x0&t=1304s
UCI Math 113B: Intro to Mathematical Modeling in Biology (Fall 2014)
Lec 20. Intro to Mathematical Modeling in Biology: Chemical Kinetics: Mass Action Law

https://www.math.utah.edu/~keener/books/control.pdf

2. RK4 code ref:
https://perso.crans.org/besson/publis/notebooks/Runge-Kutta_methods_for_ODE_integration_in_Python.html#Runge-Kutta-method-of-order-4,-%22RK4%22