kMATH 212
Lab: Mathematical modeling of enzyme kinetics
Due: end of class on the day assigned (see Course Schedule in Syllabus)
Estimated Time: 1 hour

NAME:

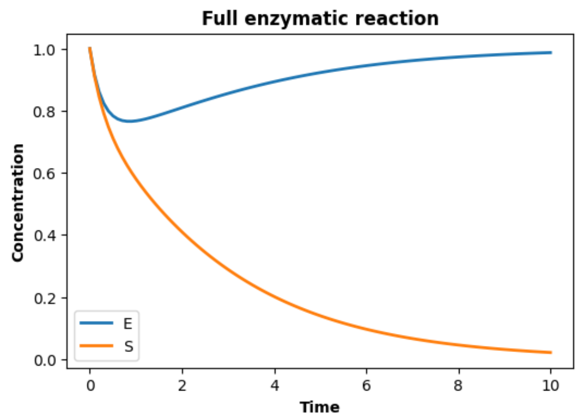
Directions: Write your answers next to the “Ans” prompts. Submit to Google classroom by clicking the “Turn In” button by the end of class.

Grading: There are 25 points possible in this lab, with points noted next to the prompt for each question you respond to.

- See the Rubric for Labs in the Google classroom Lab assignment!
- You may discuss responses as a group, but each individual must refine the work and submit their own version of the lab, containing their own spreadsheet solutions, explanations and their own handwritten work for each part.
- The explanations and mathematical work must give evidence of mastery - this is more likely with complete sentences, few or no errors, and clear concise solutions including some words rather than only numbers or symbols.
- Revisions are accepted, up to 1 week after receipt of your grade; see syllabus.

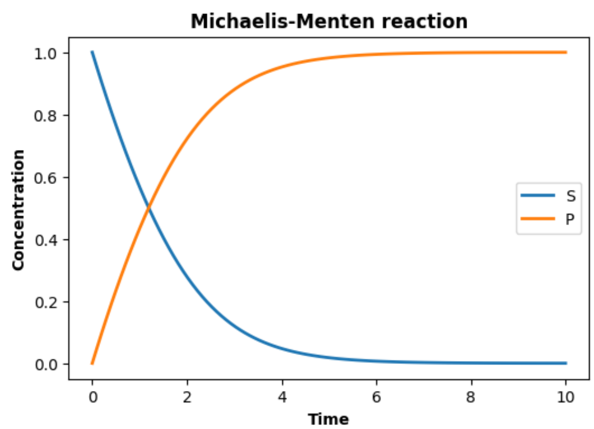
Part 1: Enzyme kinetics analysis

1. (2) Change the code simulating the original enzymatic reaction in code block #1 to plot only substrate and enzyme by changing the variables in "selections" in this line of code: `result = r.simulate(0, 10, 100,selections=['time','E','S','ES','P'] ).` Copy and paste the plot here:



2. (2) Now we will use the simplified model, the Michaelis-Menten rate law, in the code block #2. Notice that now there is only one reaction, R1, described in the code. This is the longer timescale reaction where substrate goes to product at the Michaelis-Menten rate.

   Execute this code block and copy and paste the resulting plot here:

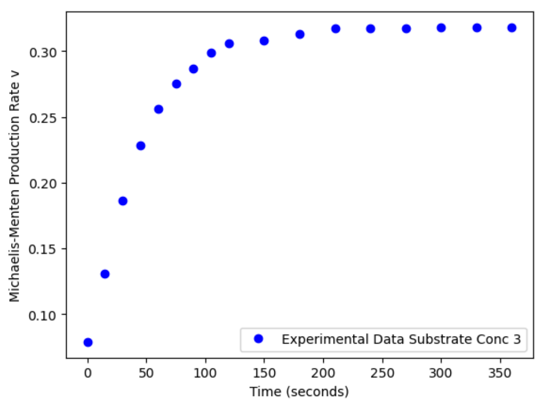


3. (3) Compare the two plots. What do you notice about the original model of the full multi-step enzymatic reaction versus the reduced version of the reaction based on the Michaelis-Menten rate law we derived?
The reduced version simplifies the four rate-of-change equations into one formula that changes ‘E’ into total E - ES and then also simplifies ES, knowing that it’s a steady state. The concentration of substrate increases inversely to the concentration of the product, simplifying the equation to only terms of substrate and product.

Part 2: Experimental data and estimated parameters v_{max} and K_M

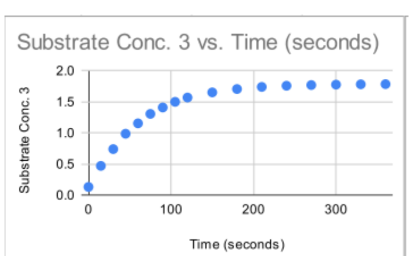
For this step, you will import your experimental data using Python and plot
.

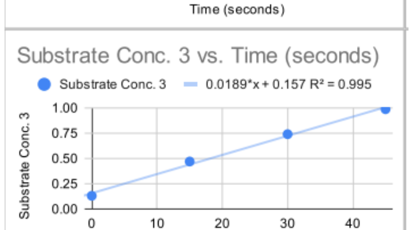
1. (3) Input your experimental data into the `time` and `rate_v` arrays in code block #4 and execute the code to import your data. If you did not complete the chemistry lab, use data from a classmate and cite whose data you use.
   Next, generate a plot of the experimental data and paste here:



2. (3) Explain the data: what does rate v represent? What is it the rate of change of?
V represents the rate of catalysis of the enzyme. V varies with teh concentration of the substrate.

3. (3) In the chemistry lab, a reciprocal transformation was applied to the substrate concentration and production rate data to obtain a linear relationship between these variables.



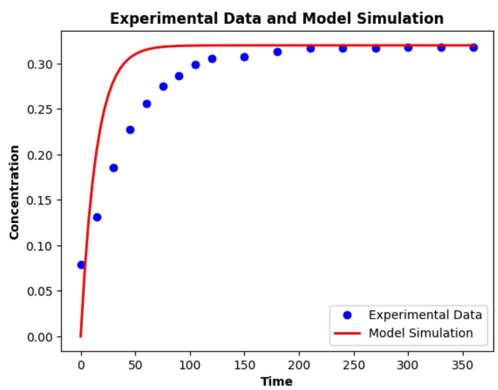


Then, linear regression allowed parameters v_{max} and K_M to be estimated from the data, by finding the best-fit line that minimizes the difference between the mathematical model and experimental data.

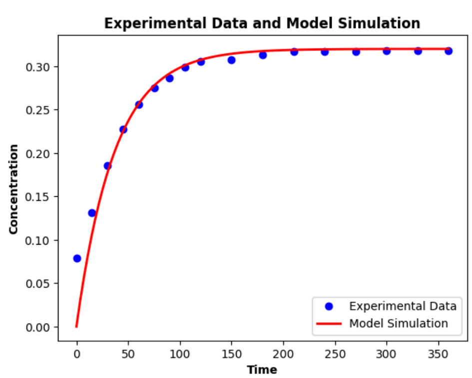
In this step, we will change the values of these parameters in the code to the values you estimated, and compare model simulation results to the experimental data.

In the code block #5, change the values of parameters vmax and KM to the values you estimated. If you did not complete the chemistry lab, use data from a classmate and cite whose data you use.

Paste the resulting graph here.



4. (3) It's likely that the model is not currently a good fit. You will need to adjust each parameter and re-graph iteratively, to try to improve the fit. Note how altering vmax changes the plot, and note how altering KM changes the plot. Recall what each of the variables represents, and **discuss whether your results make sense, and paste a plot that is the result of your best fitting efforts:**



Trends: As I increased my Vmax, it shifted the model curve more to the right. Decreasing substrate lowered the area on the curve that is flatenned. Decreasing the KM shifted the exponential area on the curve to the right. It makes sense.

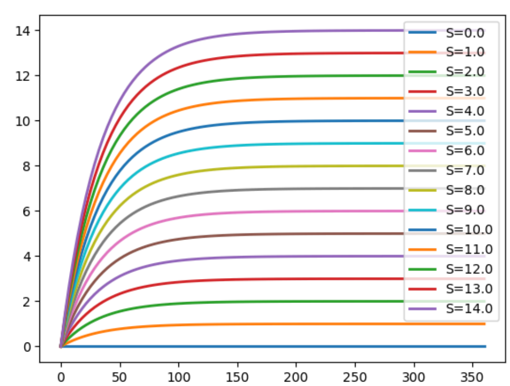
Vmax represents the maximum rate achieved; it's the maximum velocity at which the enzyme converts the substrate into the product. In my graph, Vmax is set to 70, meaning that the enzyme can process the substrate at a maximum rate of 70 units per time unit. Km is the substrate concentration at which the reaction rate ifs half Vmax. For my graph, Km is set to 2600, meaning that the enzyme reached half of its maximum reaction rate at a substrate concentration of 2600 units. The curve shows how the reaction rate increases rapidly with substrate concentration and then plateaus, representing the enzyme's limited ability to process the substrate. The Km is higher which means that it has a lower affinity for the substrate, meaning that it needs a higher concentration of substrate to achieve maximum reaction velocity.

Part 3: Simulating experiments

5. (3) A primary benefit of simulation is the ability to test hypotheses and run experiments instantaneously and without the need for reagents and assays.

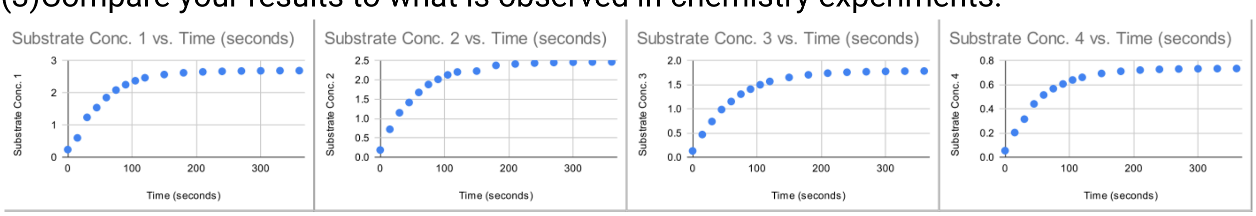
   Vary the amount of initial substrate over a wide range, and observe the impact on model predictions using code block #6.

   Paste a plot of your results:



   As the initial substrate concentration is increased, the model gets higher and higher (the Km also increases).

6. (3)Compare your results to what is observed in chemistry experiments:



   Same or different? Does changing the initial amount of substrate impact the time it takes for the reaction to reach maximum production of product, and does this match experimental observations?

Mostly the same. As the substrate concentration is increased, the time it takes for the reaction to reach Vmax also increases, which can be seen in the experimental observations as well. The time it takes for substrate concentration concentration four to max out is ~180 seconds, while in the graph for substrate concentration 2 it is much closer to 210 seconds. Interestingly though, for substrate concentration 1, which has the highest concentration, Vmax is reached around 190 seconds, showing how at some point, adding more substrate doesn't impact the Vmax as the enzyme is already saturated.