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

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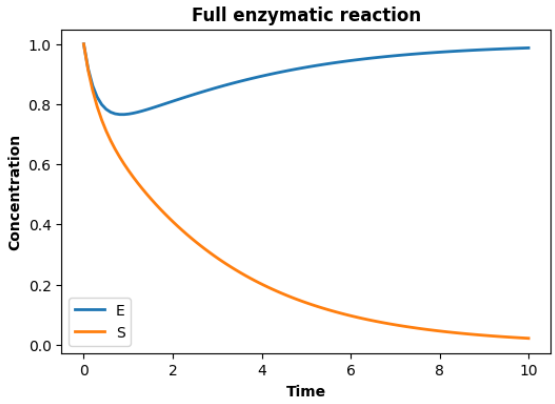
Directions: Write your answers next to the "Ans" prompts. Submit to Google classroom by clicking the "Turn In" button by the end of class.

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.

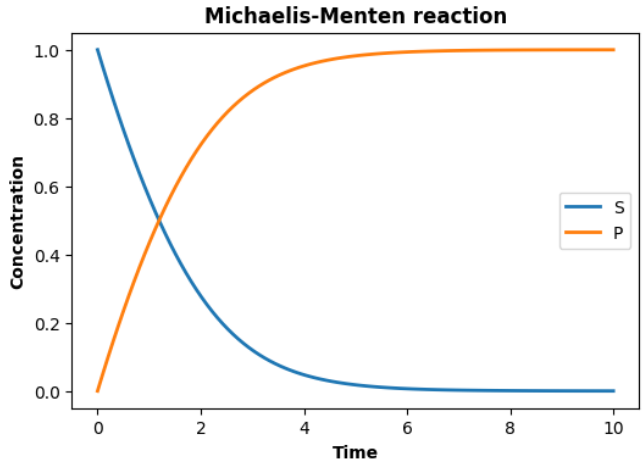
Part 1: Enzyme kinetics analysis

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:



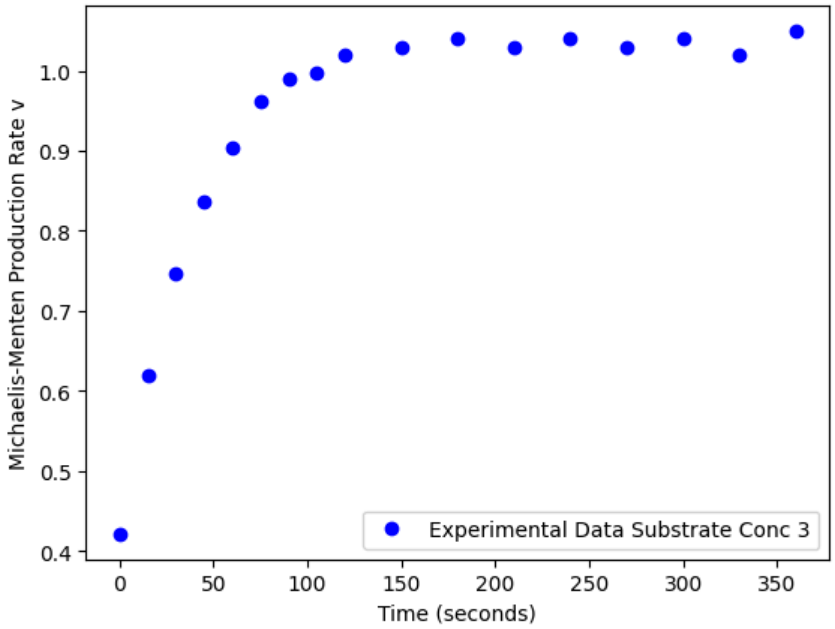
3. (3) Compare the two plots. What do you notice about the original model of the full multi-step enzymatic reaction versus the reduced version of the reaction based on the Michaelis-Menten rate law we derived?
   This proposes a new rate law and simplifies the four derivative equations into one Michaelis Maten. The first graph shows enzyme and substrate concentration while the second graph displays substrate and product. The substrate concentration decreases at relatively the same rate between the two graphs; however the second plot lines are different. The enzyme in graph one begins and ends around the same concentration while the concentration of the product increases through the reaction in graph 2.

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

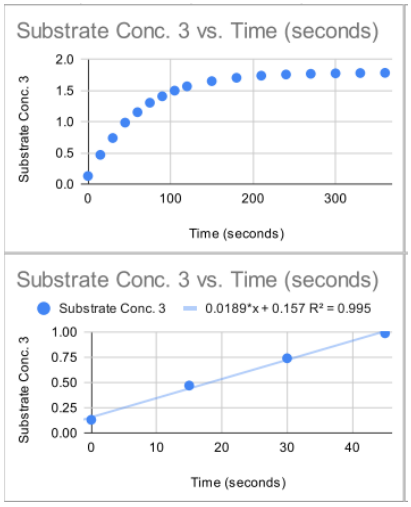
.

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 product produced as the reaction time progresses

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.

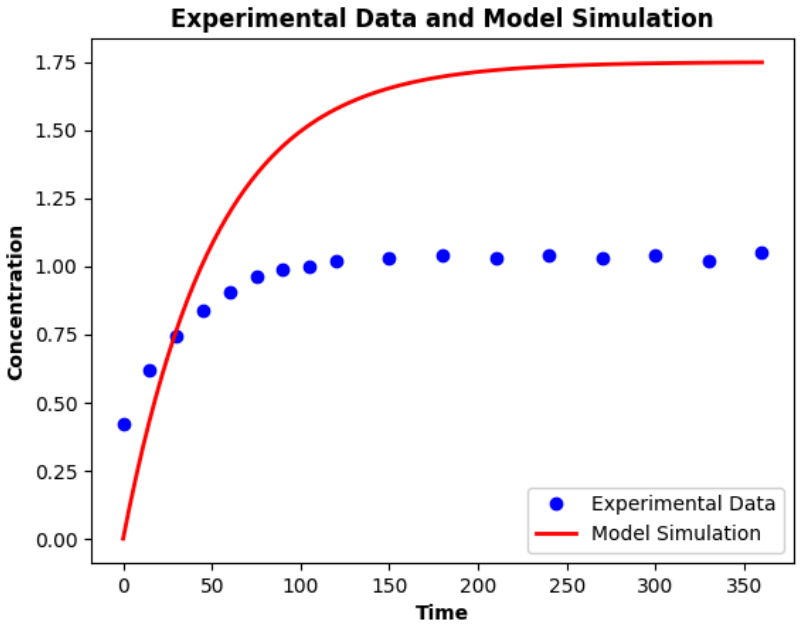


Then, linear regression allowed parameters v_{max} and K_M to be estimated from the data, by finding the best-fit line that minimizes the difference between the mathematical model and experimental data.

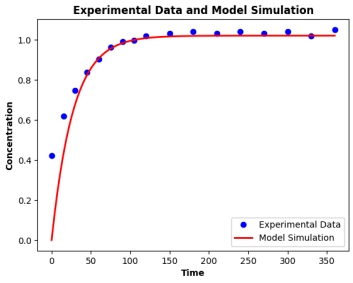
In this step, we will change the values of these parameters in the code to the values you estimated, and compare model simulation results to the experimental data.

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:**



I think these results make sense as the model simulation line follows the experimental data pretty closely. Increasing the Vmax made the curve more steep and increasing the Km shifts the graph more to the left. The parameters below are what is fiddled with to get the line closest to the data, but honestly, I am not sure these results make sense. The Km (50) makes sense since that is half of Vmax which looks like 1.00. But to make the line fit the best I had to set the Vmax to 1.85 which seems a little high.

```
S = 1.02
P = 0.0
```

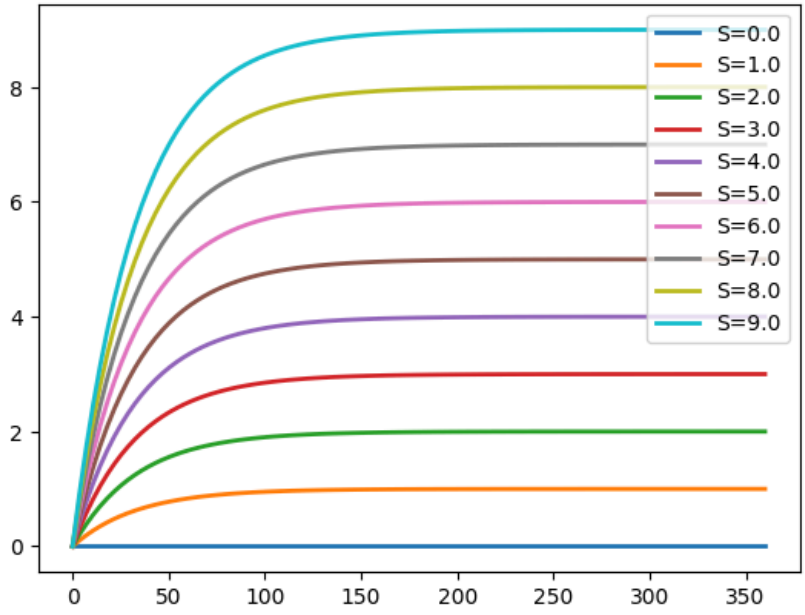
```
vmax = 1.85
K_M = 50
```

Part 3: Simulating experiments

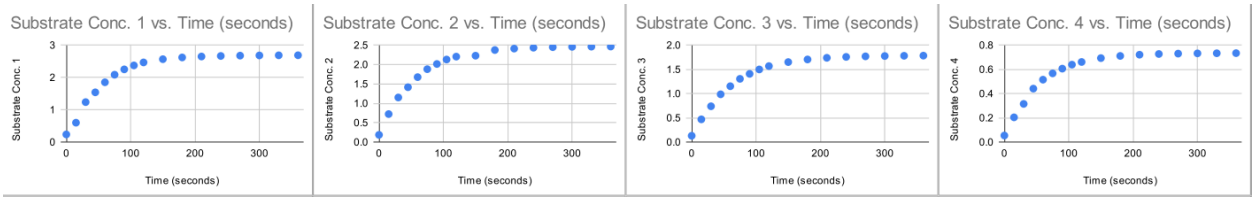
5. (3) A primary benefit of simulation is the ability to test hypotheses and run experiments instantaneously and without the need for reagents and assays.

   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:



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?

The more substrate present in the solution, would increase the amount of product produced per second to a point. Eventually, there reaches a point where all the substrate is saturated by enzyme and the rate plateaus, and adding more substrate would not impact the reaction unless more enzyme is also added. This is called Vmax. That being said, more substrate allows for a higher ceiling of product, but does not always increase the rate at which the reaction occurs. The experimental data matches this result.