ECH60 Project 3
Glycolysis Visualization
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Intro:

The objective of this project is to accurately model the biochemical process of Glycolysis which describes the way cells process sugars to release energy, forming Adenosine Triphosphate (ATP). In this project, the main portion of the glycolytic process being examined is known as Glycolytic Oscillation, which relates the behavior of ATP and Fructose-6-phosphate (F6P). The parameters of the calculation include the concentrations of ATP and F6P as well as kinetic constants that are temperature dependent, here known as a and b. Finally, as this is an equilibrium process, time was used to show the behavior of the concentration over an extended period. All of these parameters were used in equations (1) and (2) to model this behavior and allow for the visualization as seen in the following plots. Part 3 added an additional equation (3) to model the behavior of the kinetic constant b over time.

Equations:

$$\frac{d[ATP]}{dt} = -[ATP] + a[F6P] + [ATP]^2[F6P] \quad (1)$$

$$\frac{d[ATP]}{dt} = b - a[F6P] - [ATP]^2[F6P] \quad (2)$$

$$\frac{db}{dt} = -0.1[F6P][ATP]e^{-1/b} \quad (3)$$

Pseudo-Code:

- Constant parameters (a and b) and initial conditions ($[ATP]_0$ and $[F6P]_0$)
- Define differential functions for [ATP] and [F6P]
- Create a time range and blank solutions of same length
- Simultaneous Runga-Kutta 4 for [ATP] and [F6P]
    - Part B required an 'if' statement for t = 30
    - Part C required a separate function for the parameter b, as well as an initial condition and an RK4 for it

Results and Conclusion:

The steady state concentrations in Part A do not depend on the initial conditions. Changing the initial concentrations does not change the fact that the concentrations equilibrate. This is further shown in Part B as the b parameter changes and the concentrations do not reach steady state within 100 time units. The change in the b parameter in Part B leads to glycolytic oscillations.

In Part C, the b parameter is varied as time t varies. Similarly to Part B, the concentrations of ATP and F6P appear to oscillate for some time. However, as time progresses, both of the concentrations trend to a steady state. Furthermore, the steady state behavior that is exhibited with the given parameters in this part is not dependent on the initial conditions, so any variation of the initial conditions will result in the same steady state behavior. The only challenge that was encountered in this project was effectively visualizing the results for each part. Without proper visualization, it would be difficult to interpret the results correctly.

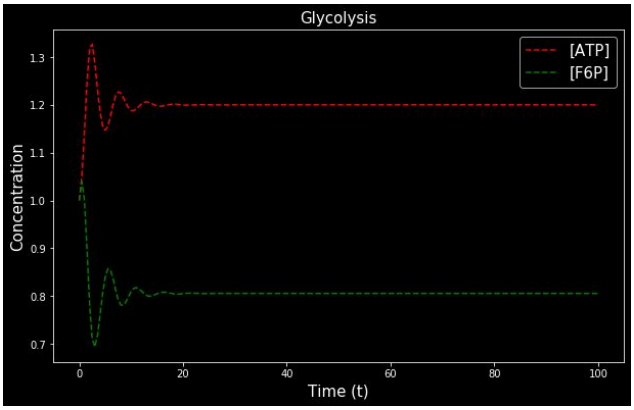

Figure 1: Steady State Equilibrium Behavior

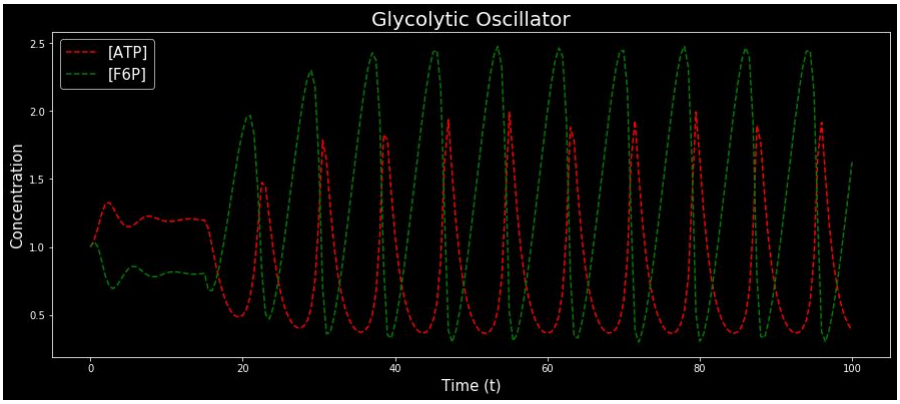

Figure 2: Glycolytic Oscillator

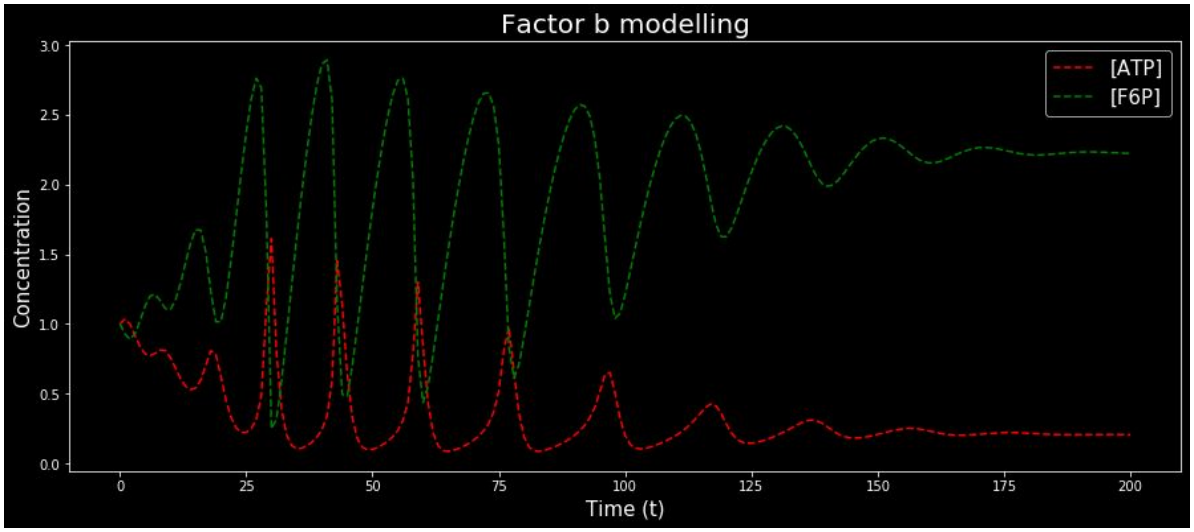

Figure 3: Glycolytic Oscillator with factor b accounted for

References: ECH60 Lectures and Slides, ECH60 Jupyter Notebook Tutorials