Numerical Methods Applied to an Enzyme Kinetics Model

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Abstract

In this work, we study enzyme kinetics using numerical techniques, such as Euler's Method and Taylor's Series Method. Our system consists of four ordinary differential equations, each of them describing the reaction rate of specific compounds in reaction. We represent the numerical solution and plots of each reactant using MATLAB program. We compared the performance of our numerical methods with methods used in Callie Martins' Enzyme Kinetics Spring 2012 Work.

Background

Enzymes are biological substances in charge of decreasing the energy necessary for a reaction to occur. Because they lower this activation energy and speed up a reaction without being consumed themselves, we called them biological catalysts. Chemical kinetics is the study of the rates of chemical reactions, where enzyme kinetics is the study of how biological catalysts increase the reaction rate in biochemical reactions. Rates are dependent on the concentrations of reactants.

$$\text{Rate} = k\,[\text{Reactant}]^n$$

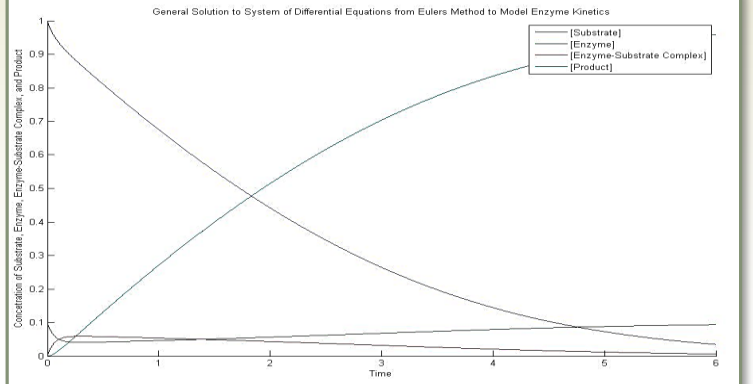
This expression is called a rate law where the rate constant k and the order of the reactant n are determined experimentally.

Rate Equations

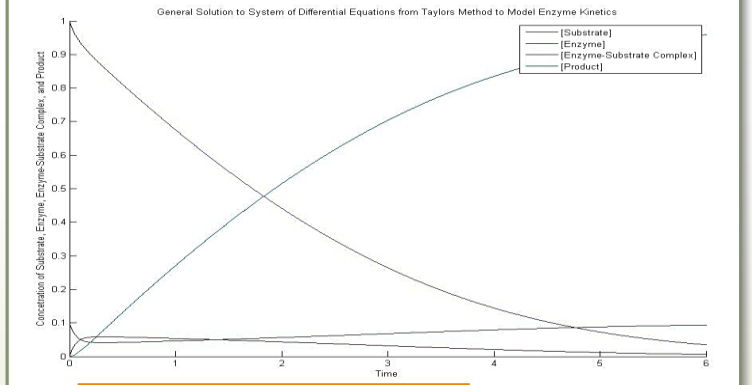
Our system is given by four differential equations describing the rates for specific compounds in reaction:

Substrate	$S' = -k_1 E.S + k_2 C$
Unoccupied Enzyme	$E' = -k_1 E.S + k_2 C + k_3 C$
Enzyme-Substrate Complex	$C' = k_1 E.S - k_2 C - k_3 C$
Product	$P' = k_3 C$

Results



Euler's Method



Taylor's Method

Norm

For $h = 0.001$,

	Taylor	Euler
Substrate	1	1
Enzyme	0.1000000000000	0.1000000000000
Enzyme-Substrate Complex	0.0590875055273	0.0591071175369
Product	0.9590454904099	0.9590827242591

Numerical Methods

- **Euler's Method**

To approximate the solution of the initial-value problem, $y' = f(x,y)$, $y(x_0) = y_0$, we use a positive increment h on the x-axis. Then, we can find a point $(x_1, y_1) = (x_0+h, y_1)$ on the tangent line to the unknown solution curve at (x_0, y_0). If we label x_0+h by x_1, the point (x_1, y_1) on the tangent line is an approximation to the point $(x_1, y(x_1))$. In general, it follows that $y_{n+1} = y_n + hf(x_n, y_n)$ where $x_n = x_0 + nh$.

- **Taylor Series Method of Order Two**

To study numerical solutions, we use the Taylor's series expansion centered at a point $x = x_n$ for a function $y(x)$ that possesses derivatives of all orders. We have that

$$y(x_n + h) = y(x_n) + y'(x_n)h + \frac{y''(x_n)h^2}{2} + \cdots$$

If we truncate the series two terms and we use the same approximation used in the Euler's method, it follows that $y_{n+1} = y_n + y'_n h + y''_n \frac{h^2}{2}$ where y'' is obtained by differentiating $y' = f(x,y)$.

Conclusion

By analyzing the results and norm from both methods, we can conclude that the Taylor's method is more accurate than the Euler's method since it is O (h^2) while Euler's method is O (h). For Taylor series method of order 2, the error decreases more quickly by reducing the value of h thus giving a more accurate rate of reactions for each specific compound in reaction.

References

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Zumdahl Steven, and Zumdahl Susan. *Chemistry, 9th Edition.* Belmont: Cengage, 2014. Print.