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Mathematical treatment of Enzyme Kinetics using differential method

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ABSTRACT

In this article, we studied the theoretical investigation of basic enzyme reactions of substrate and product concentrations. The enzyme kinetics helps in drug designing, Drug Metabolism and the determination of disassociation constants for antigen-antibody interactions in solutions. The arising physical governing system we solved by using the general ordinary differential method. The obtained results show the substrate, enzyme, substrate-enzyme and product concentration profiles are presented with help of graphs and tables. From this study we found that as increasing substrate value improves the rate of reaction. If the rate constant is greater than substrate concentration, then rate of reaction depends on free enzyme content and substrate amount. In the similar way, the substrate concentration is greater than rate constant the rate of reaction depends only on free enzyme content.

Keywords: *Enzyme, Substrate, Differential transform method, rate constant, Kinetics.*

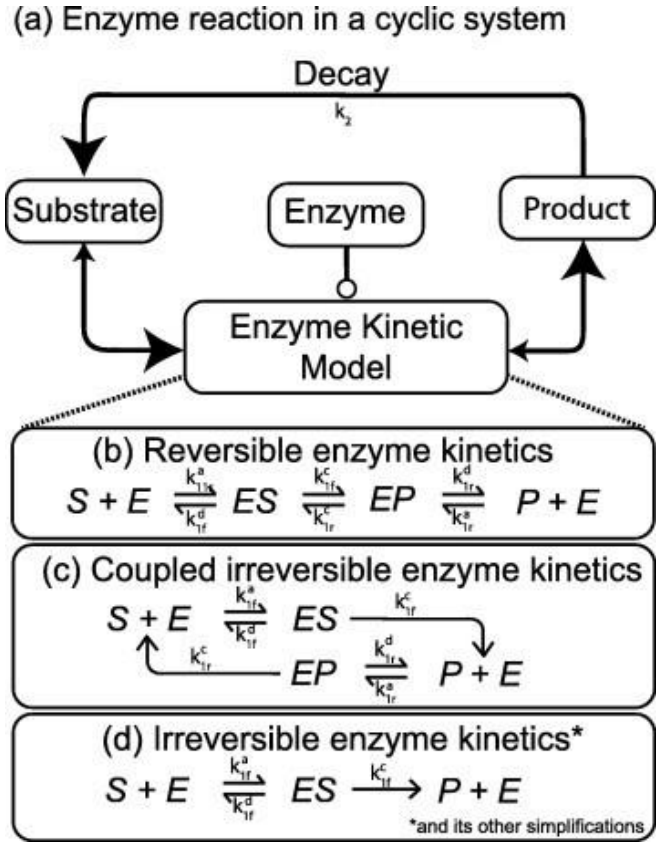
1. INTRODUCTION

Recently, the various reactions that are carried in our cells are influenced by enzymes which acts like catalyst that never involve in any reaction but influences the rate of reaction. Enzyme kinetics involves the rate of many processes such as a) Inhibition is the process which enzyme behaves as negative catalyst and makes the reaction slowly. b) Substrate breakdown, in this the enzyme will divide the complexes. c) Substrate binding, in this the enzyme binds the complexes into a single complex and selective enzyme kinetics which impacts drug metabolism. Enzymes not only limited to these processes but also helps in DNA translating, energy production, in which enzymes generates ATP molecules that gives power to your cells. Enzymes can be classified on the basis of the reaction in which they are going to catalyse. One such classification is made by IUBMB (INTERNATIONAL UNION OF BIOCHEMISTRY AND MOLECULAR BIOLOGY) [1]. Enzyme kinetics are used in the leather manufacturing, textile industry, baking, and determination of detergent action on laundry, and many more [2]. To know more about enzyme kinetics researchers has to enhance the rate reactions and the conditions which influence enzyme kinetics. Our investigation uses the linear differential equations gives the approximate relation between enzyme, substrate, enzyme substrate complex, product and their rates. This relation is already given by Michaelis –Menten [3] using algebraic form but we reduced it to differential equations. The relation is given by.

$$v = \frac{V_{\max} s}{K_m + s} \qquad (1)$$

The study of enzyme kinetics gives the knowledge of rate reactions. So, accordingly we can manipulate concentrations in order to increase or decrease the rate of a reaction. From (1) the V_{max} gives the maximum rate of a reaction, s gives the concentration of substrate and K_m gives the Michaelis constant.

2. ENZYME ACTION



3. METHODOLOGY

Let the simplified reaction be

$$S + E \underset{k_2}{\overset{k_1}{\rightleftarrows}} SE \underset{k_4}{\overset{k_3}{\rightleftarrows}} P + E \qquad (2)$$

at very low concentration product concentration is very less and the reversible reaction is not feasible. So we neglect the reversible reaction from P + E to ES. So now the reaction becomes

$$S + E \underset{k_2}{\overset{k_1}{\rightleftarrows}} SE \xrightarrow{k_3} P + E \qquad (3)$$

k_1 be the rate constant of the reaction from S + E to SE k_2 be the rate constant of the reaction from SE to S + E and k_3 be the rate constant of reaction from SE to P + E.

let us consider the concentrations be
[S] = s, [E] = e, [ES] = c, [P] = p

$$\frac{ds}{dt} = k_2 c - k_1 se$$

$$\frac{de}{dt} = - k_1 se + (k_2 + k_3)c$$

$$\frac{dc}{dt} = - k_2 c - k_3 c + k_1 se$$

$$\frac{dp}{dt} = k_3 c$$

conservation of mass for enzyme

$$\frac{de}{dt} + \frac{dc}{dt} = 0$$

integrating with respective to time(t)

$$\int \frac{de}{dt} + \int \frac{dc}{dt} = \int 0$$

we get e(t)+c(t)=constant
taking boundary conditions i.e., at time t=0 c(0)=0
we get constant = e_0.

then $e(t)=e_0-c(t)$.
then

$$\frac{ds}{dt} = k_2 c - k_1 s[e_0 - c]$$

$$\frac{dc}{dt} = -k_2 c - k_3 c + k_1 s[e_0 - c]$$

quasi steady state approximation: after a short period of time in which the enzyme 'fills up' the amount of complex c stays almost the same.

$$\frac{dc}{dt} = 0$$

$$-k_2 c - k_3 c + k_1 s[e_0 - c] = 0$$

$$c = \frac{se_0}{k_m + s}$$

where $k_m = \frac{k_2 + k_3}{k_1}$

$$\frac{ds}{dt} = -k_1 s[e_0 - c] + k_2 c$$

substituting c in above equation

$$= -k_1 s e_0 + [k_1 + k_2]\frac{se_0}{k_m + s}$$

$$= [k_2 - k_1 k_m]\frac{se_0}{k_m + s} \quad \text{let } k = k_2 - k_1 k_m$$

$$= k\frac{se_0}{k_m + s} \quad \text{where } ke_0 = v_{max}$$

$$v = \frac{v_{max} s}{k_m + s} \qquad (4)$$

where v gives the rate of reaction.

v_{max} gives the maximum rate of the reaction.

s gives the substrate concentration.

k_m gives the Michaelis Constant.

4. RESULTS AND DISCUSSIONS

The equation (4) and equation (1) which was proved by Michaelis Menten equation resembles the same so the differential approach is also favourable.
From the equation (4) there are two conditions:

$$(i)\ if\ k_m \gg s\ :$$

$$v = \frac{v_{max} s}{k_m} \qquad (5)$$

From equation (5) it's clear that rate only depends on the substrate amount and the free enzyme content (e_0) as k_m is constant.

$$(ii)\ if\ s \gg k_m :$$

$$v = \frac{v_{max} s}{s} = v_{max} \qquad (6)$$

From equation (6) it's clear that rate only depends on the free enzyme content.

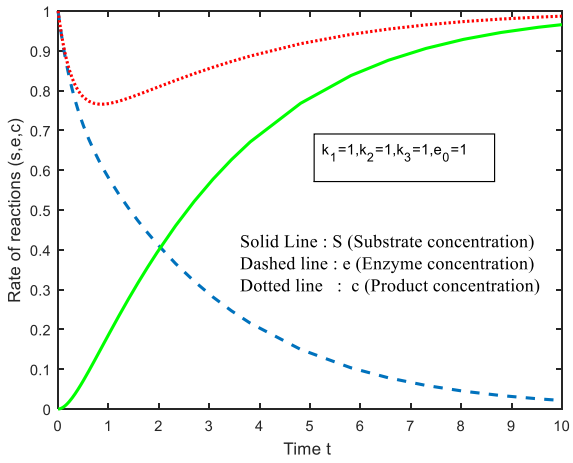


Fig. 1 Rate of reaction with time *t*

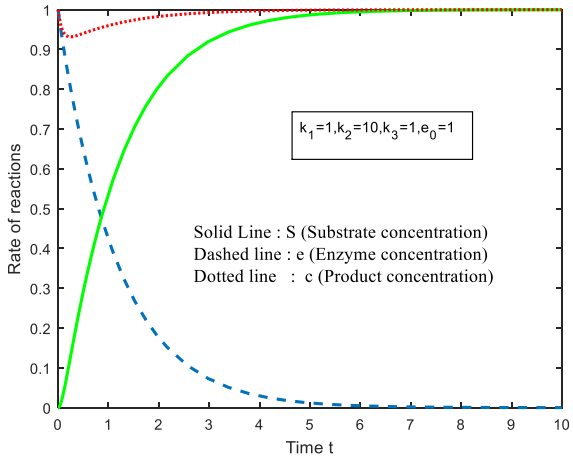


Fig. 2 Rate of reaction with time *t* when k_2 =10

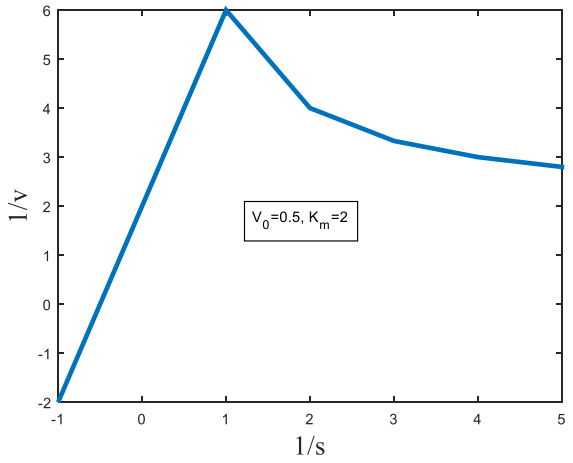


Fig. 3 1/s versus 1/v

From the depicted graphs it is shown that with increase in time the rate of reaction increases. [4]
Because of molecular collisions rate of reaction varies increase in molecular collisions decreases electron affinity which increases rate of a reaction. [5]

5. CONCLUSIONS

In summary,

- Enzyme Kinetics helps in the determination of disassociation constants for antigen – antibody interactions in solutions.
- According to researchers Double reciprocal plots of Elisa signals Vs Antigen Concentration helps in Studying Antigen-Antibody binding and hence Aids Drug designing and also the study of Drug Metabolism.
- It is used in Cancer Therapy, it has an industrial application.

6. REFERENCES

[1] https://chembioinfo.com/2011/03/03/how-are-enzymes-classified/
[2] http://www.mapsenzymes.com/enzymes.asp
[3] http://www.ou.edu/OpenEducation/ou-resources/biochemical-methods/lab-11/michaelis-menten-derivation.pdf .
[4] JOHN E. "*A comparison of estimates of Michaelis-Menten Kinetic Constants from various Linear transformations"* The journal of Biological Chemistry Vol.240, No.2, February 1965.
[5] https://www.chemguide.co.uk/physical/basicrates/introduction.html

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