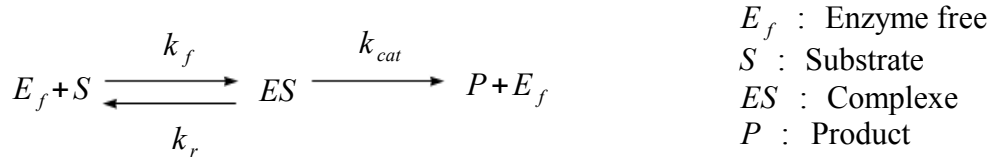


**ABSTRACT**

To measure enzyme kinetics model of a catalytic base where an enzyme E reacts with a substrate S to form a complex ES. The ES complex can be dissociated: either by one enzyme molecule E with one substrate molecule S or either one enzyme molecule E with one product molecule P; we can use the model established by Michaelis and Menten.



$k_f > 0$ ,  $k_r \geq 0$  and  $k_{cat} > 0$  are the rate constants of the different reactions.

- $k_f$  : kinetic forward constant
- $k_r$  : kinetic reverse constant
- $k_{cat}$  : kinetic catalytic constant

The rate of the enzymatic reaction ( $v$ ) is the rate of the occurrence product.

$$v = \frac{dP}{dt} = k_2 [ES](t)$$

If the substrate concentration is infinite, all the free enzyme form ES complex.

**Now, if  $[E_f] = [E_{total}]$  so  $v = v_{max}$ .**

$$v_{max} = k_2 [E_{total}]$$

Whether,  $\frac{v}{v_{max}} = \frac{k_2 [ES](t)}{k_2 [E_{total}]}$  and give the equation of speed :  $v = v_{max} \frac{[ES](t)}{[E_{total}]}$

**Define Michaelis Constant or  $K_m$**

To set the  $K_m$ , define steady state of  $ES(t)$

$$\frac{d[ES](t)}{dt} = 0$$

$$\frac{d[ES](t)}{dt} = k_f [E_f](t) [S](t) - (k_r + k_{cat}) [ES](t)$$

Whether,  $k_f [E_f](t) [S](t) - (k_r + k_{cat}) [ES](t) = 0$

**Michaelis constant :**  $\frac{[E_f](t) [S](t)}{[ES](t)} = \frac{k_r + k_{cat}}{k_f} = K_m$

**Define Equation of MICHAELIS - MENTEN**

It is known,  $\frac{[E_f](t)[S](t)}{[ES](t)} = K_m$  and  $[E_f](t) = [E_{total}] - [ES](t)$ . By substitution,

$$\frac{([E_{total}] - [ES](t))[S](t)}{[ES](t)} = \left( \frac{[E_{total}]}{[ES](t)} - 1 \right) S(t) = \frac{[E_{total}]S(t)}{[ES](t)} - S(t) = K_m$$

Solve,

$$\frac{[E_{total}]S(t)}{[ES](t)} = K_m + S(t) \Rightarrow \frac{[E_{total}]}{[ES](t)} = \frac{K_m + S(t)}{S(t)} \Rightarrow \boxed{\frac{[ES](t)}{[E_{total}]} = \frac{S(t)}{K_m + S(t)}} \quad (1)$$

By substitution, (1) is integrated in the equation of speed and we get **the equation of MICHAELIS - MENTEN** :

$$\boxed{v = v_{max} \frac{S(t)}{K_m + S(t)}}$$

### The numerical model of Michaelis - Menten

We can deduce the differential relation :

$$[P]'(t) = \frac{v_{max}[S](t)}{K_m + [S](t)}$$

Differential equation of the instantaneous velocity of product formation.

$$[S]'(t) = -\frac{v_{max}[S](t)}{K_m + [S](t)}$$

Differential equations of the instantaneous speed of substrate disappearance.

$$[ES](t) = [E_{total}] \frac{S(t)}{K_m + S(t)}$$

Differential equation of the instantaneous velocity of complex formation.

$$[E_f](t) = [E_{total}] - [ES](t)$$

Differential equation of the instantaneous velocity of complex disappearance or enzyme free.

We get a possible solution for this model with Euler-Cauchy method of taking a step  $h > 0$  but small enough.

As the variable  $S(t)$  is defined by the recursion :

$$\boxed{S_{i+1} = S_i - h \frac{v_{max} S_i}{K_m + S_i}} \quad (2)$$

And  $P_i$  is define by the recursion :  $P_i = P_0 + S_0 - S_i$

**Limite of Euler-Cauchy method**

For define the approximation to numerical solution of equation by Euler-Cauchy method, it is necessary to get a time step  $h$  quite small such as  $h > 0,1$  (empirical determination)

If  $h$  is not quite small, so the numerical solution for equation become a degenerate solution for  $\epsilon \simeq \lim S(t)$

**Relative error of the Eule-Cauchy method applied to the Michaelis-Menten model or Er (t)**

For everything  $t$  with two different steps, such as  $h_\alpha > h_\beta$ .

With

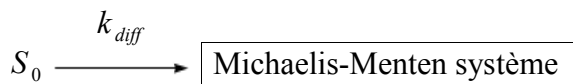
$$Er_{h_\alpha}(t) = 1 - \frac{S(t) - h_\beta \frac{v_{max} S(t)}{K_m + S(t)}}{S(t) - h_\alpha \frac{v_{max} S(t)}{K_m + S(t)}}$$

Either  $h_\alpha$ ,  $S_{i+1} = S_i - h_\alpha \frac{v_{max} S_i}{K_m + S_i}$  and for  $h_\beta$ ,  $S_{i+1} = S_{i + \frac{h_\alpha}{h_\beta}} - h_\beta \frac{v_{max} S_{i + \frac{h_\alpha}{h_\beta}}}{K_m + S_{i + \frac{h_\alpha}{h_\beta}}}$

**Integration in our model**

The product of degradation by NB-esterase 13 are ethylène terephthalic acid. Ethylene glycol diffuses into the cell plasma membrane and terephthalic acid. Terephthalic acid enter in the cell using the TPA transporter.

$S_0$ : Substrat in media glycol and through the enter in the  
 $k_{diff}$ : Diffusion constant



**Model for diffusion throug the plasma cell or  $S_{cell}(t)$**

**At the order of magnitude of cell  $S_0 = \infty$ .**

$S_{cell}(t)$  is define by addition of the diffusion constant  $k_{diff}$  at the recursion (2).

So  $S_{cell}(t)$  is define by the recursion

$$\boxed{S_{cell\ i+1} = k_{diff} + S_i - h \frac{v_{max} * S_i}{K_m + S_i}}$$