
Enzyme Reaction Simulation : Michaelis-Menten Kinetics

Introduction

Chemists are concerned with the laws of chemical interactions.

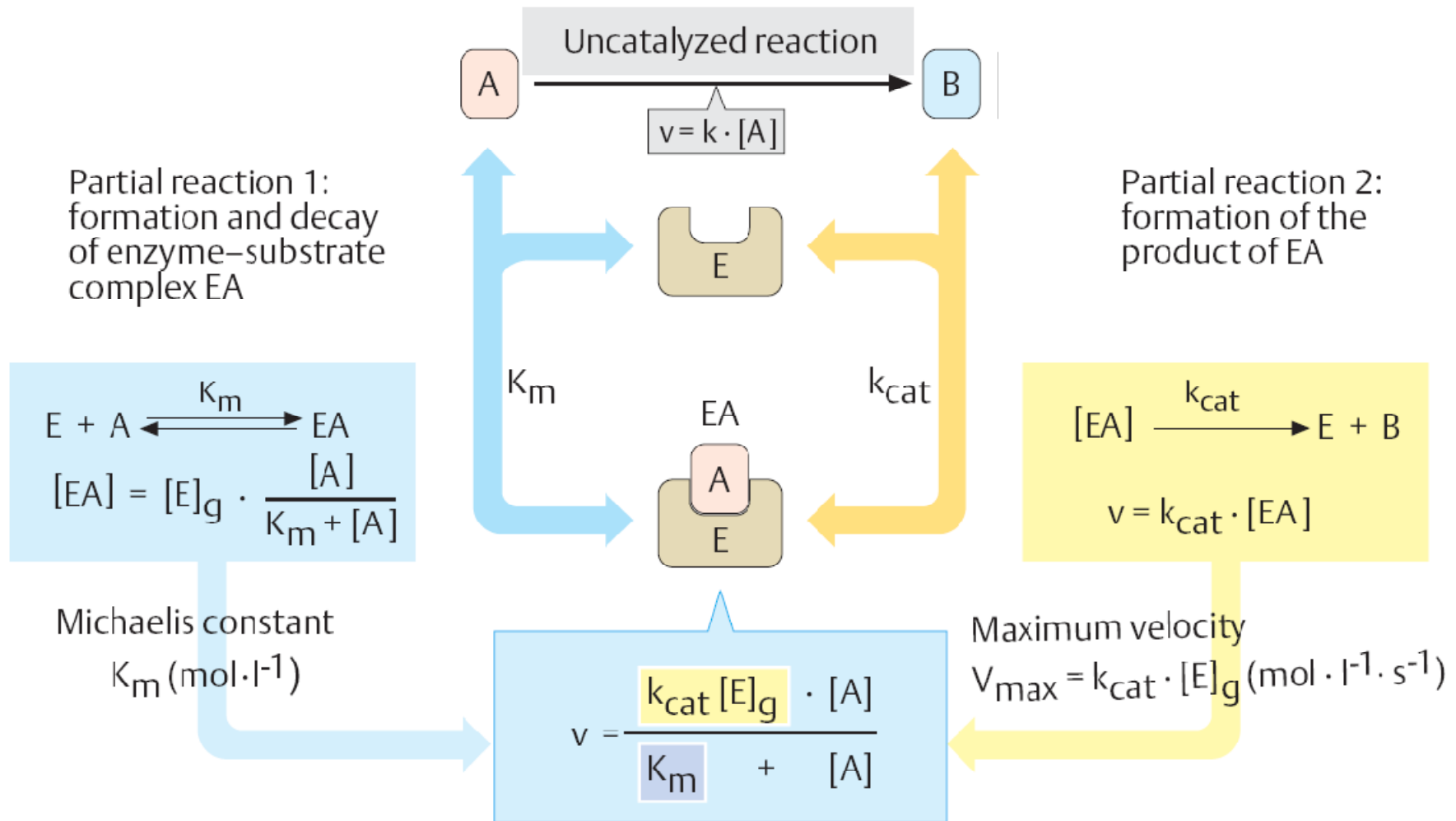
Two main approaches have been used to explain chemical reactivity: thermodynamic and kinetic. Theoretical analysis of the kinetics, or time course, of processes can provide valuable information concerning the underlying mechanisms responsible for these processes.

For this purpose it is necessary to construct a mathematical model that embodies the hypothesized mechanisms.

Whether or not the solutions of the resulting equations are consistent with the experimental data will either prove or disprove the hypothesis.

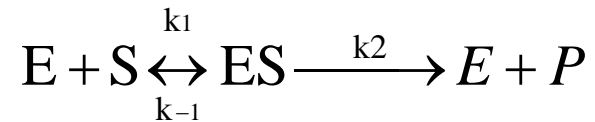
The task of a kineticist is to predict the rate of any reaction under a given set of experimental conditions. At best, a mechanism is proposed that is in qualitative and quantitative agreement with the known experimental kinetic measurements.

Michaelis-Menten Kinetics



ODEs from M-M Kinetics

Reaction Mechanism



**E : enzyme, S : substrate, P : product,
ES : enzyme-substrate complex**

$$\frac{d[S]}{dt} = -k_1[E][S] + k_{-1}[ES]$$

$$S=y_1$$

$$\frac{d[ES]}{dt} = k_1[E][S] - (k_{-1} + k_2)[ES]$$

$$ES=y_2$$

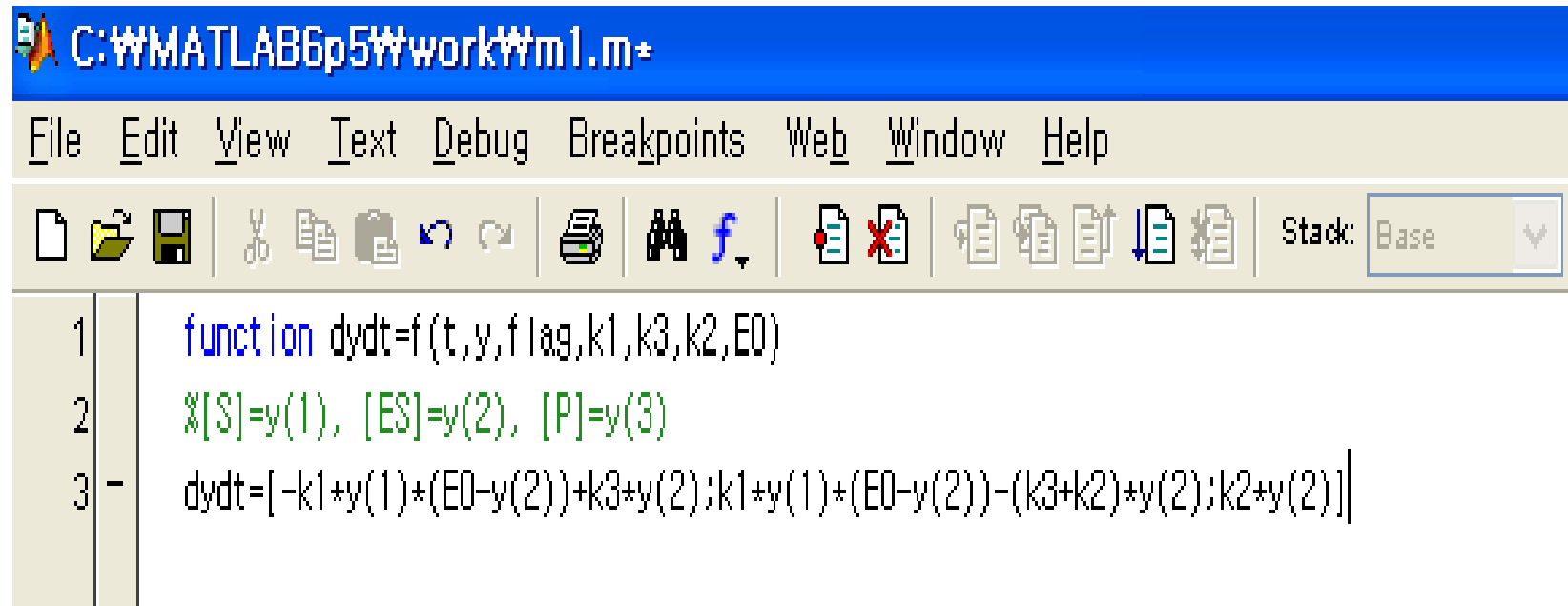
$$\frac{d[P]}{dt} = k_2[ES]$$

$$P=y_3$$

$$E=E_0-ES$$

$$=E_0-y_2$$

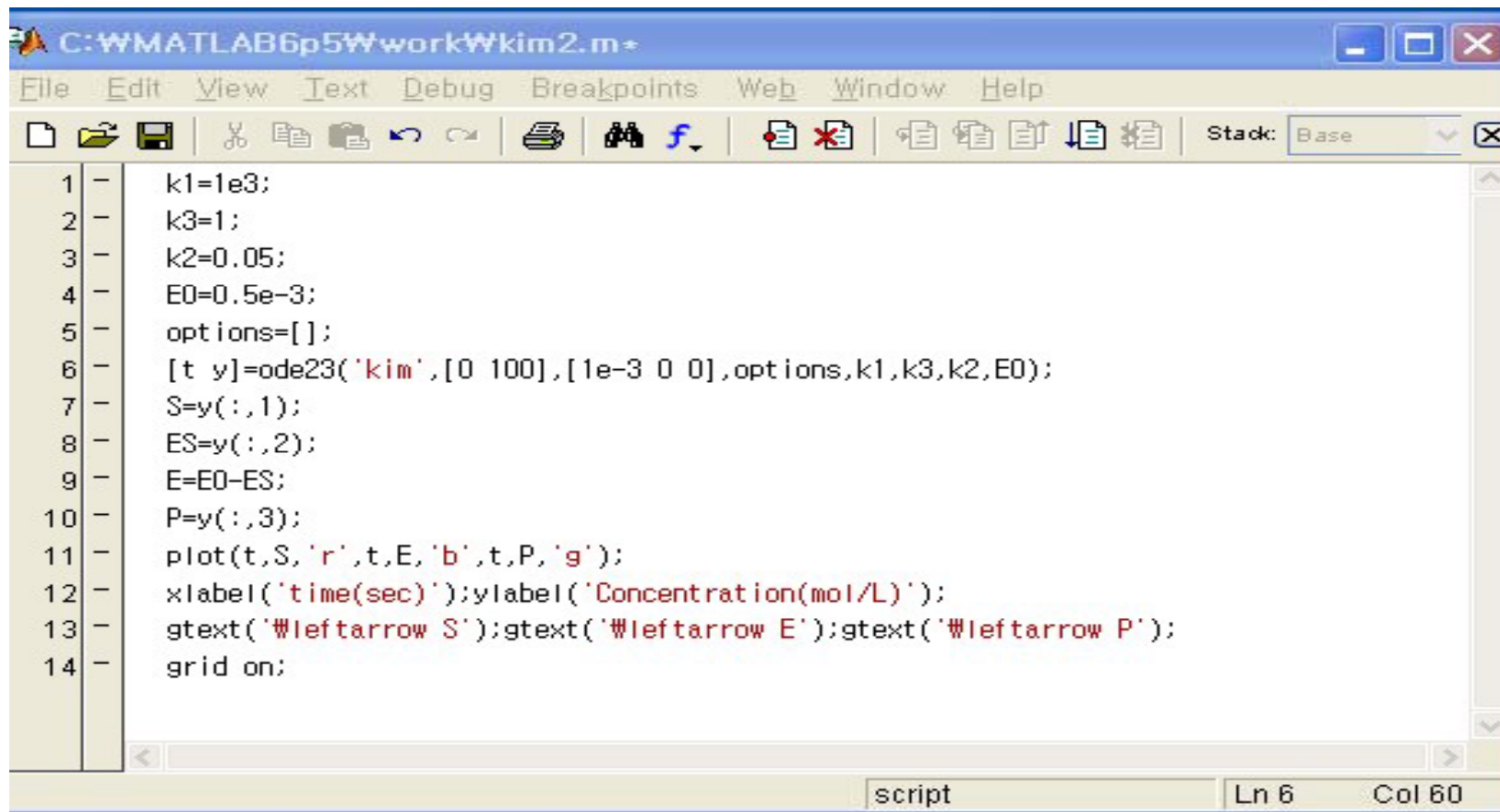
Matlab Program



The image shows a screenshot of a MATLAB editor window. The title bar reads "C:\MATLAB6p5\work\m1.m*". The menu bar includes "File", "Edit", "View", "Text", "Debug", "Breakpoints", "Web", "Window", and "Help". The toolbar contains various icons for file operations, editing, and debugging. The main editing area shows the following code:

```
1 function dydt=f(t,y,flag,k1,k3,k2,E0)
2 % [S]=y(1), [ES]=y(2), [P]=y(3)
3 - dydt=[-k1*y(1)+(E0-y(2))+k3*y(2);k1*y(1)+(E0-y(2))-(k3+k2)*y(2);k2*y(2)]
```

Program (continued)

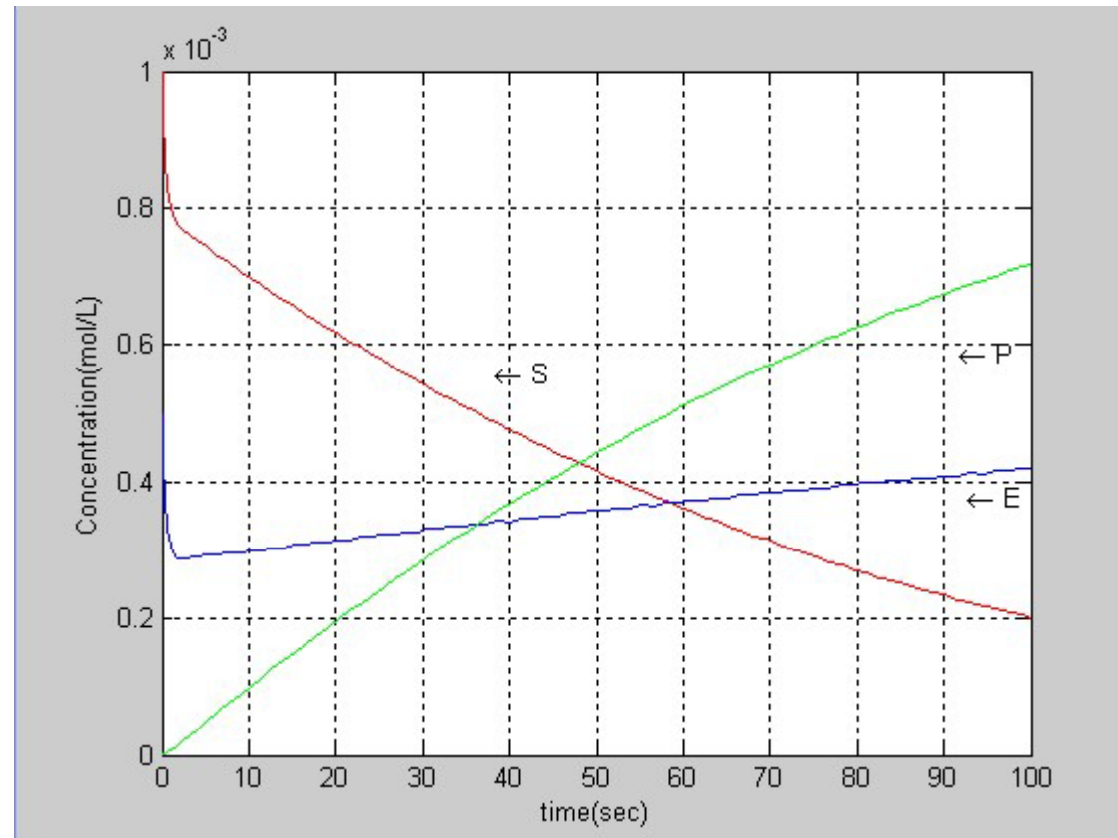


The screenshot shows a MATLAB script editor window with the following code:

```
1 - k1=1e3;  
2 - k3=1;  
3 - k2=0.05;  
4 - E0=0.5e-3;  
5 - options=[];  
6 - [t y]=ode23('kim',[0 100],[1e-3 0 0],options,k1,k3,k2,E0);  
7 - S=y(:,1);  
8 - ES=y(:,2);  
9 - E=E0-ES;  
10 - P=y(:,3);  
11 - plot(t,S,'r',t,E,'b',t,P,'g');  
12 - xlabel('time(sec)');ylabel('Concentration(mol/L)');  
13 - gtext('\leftarrow S');gtext('\leftarrow E');gtext('\leftarrow P');  
14 - grid on;
```

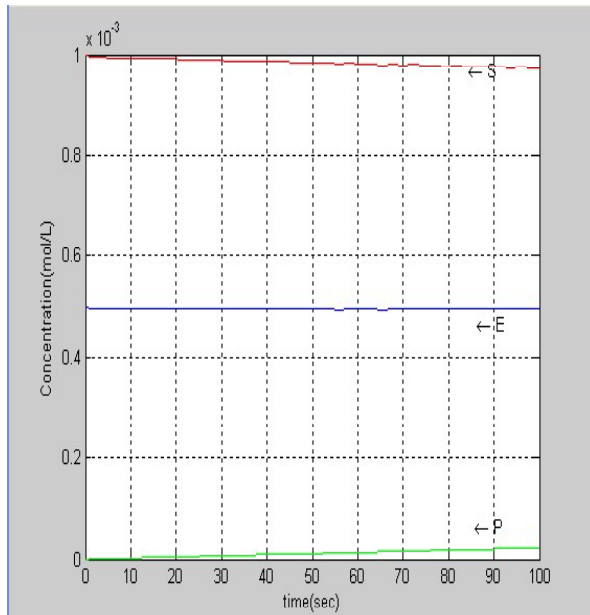
The window title is "C:\WMATLAB6p5\work\Wkim2.m". The menu bar includes File, Edit, View, Text, Debug, Breakpoints, Web, Window, and Help. The toolbar contains various icons for file operations and debugging. The status bar at the bottom shows "script", "Ln 6", and "Col 60".

Simulation Results

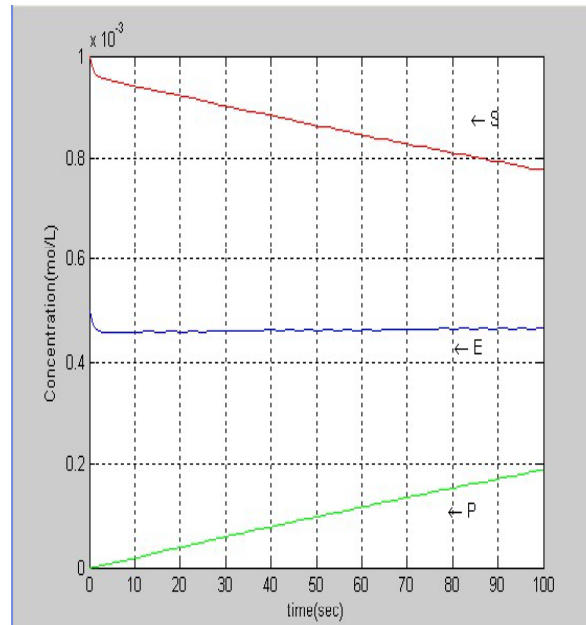


Parameter Variation

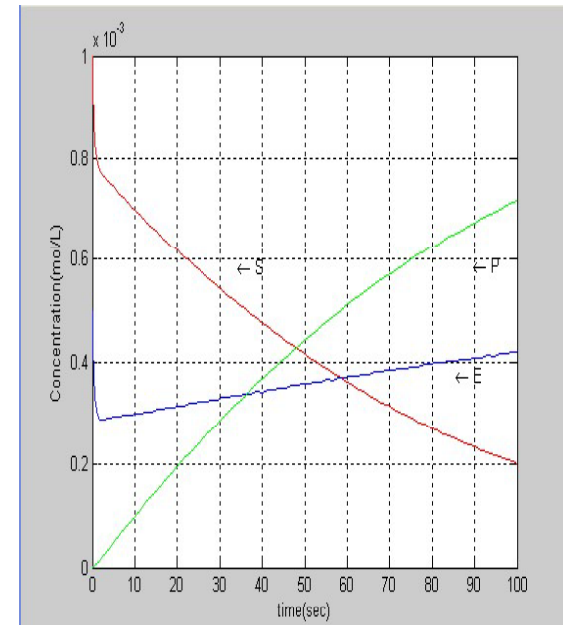
$k_1=1e^1$



$k_1=1e^2$

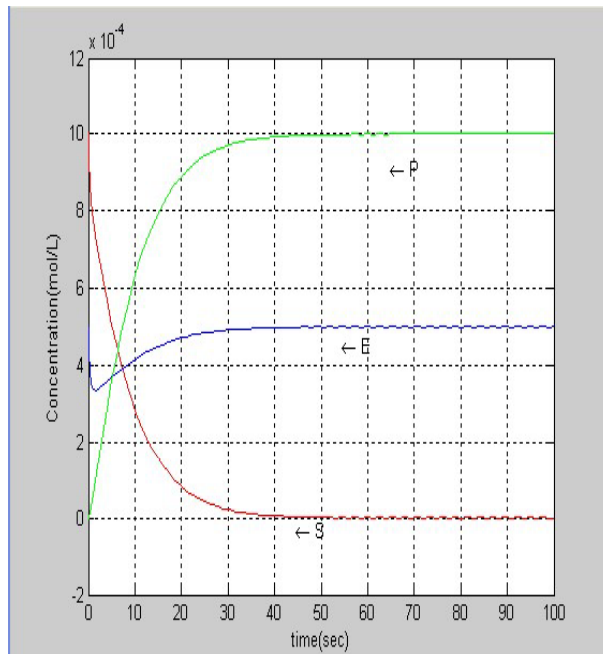


$k_1=1e^3$

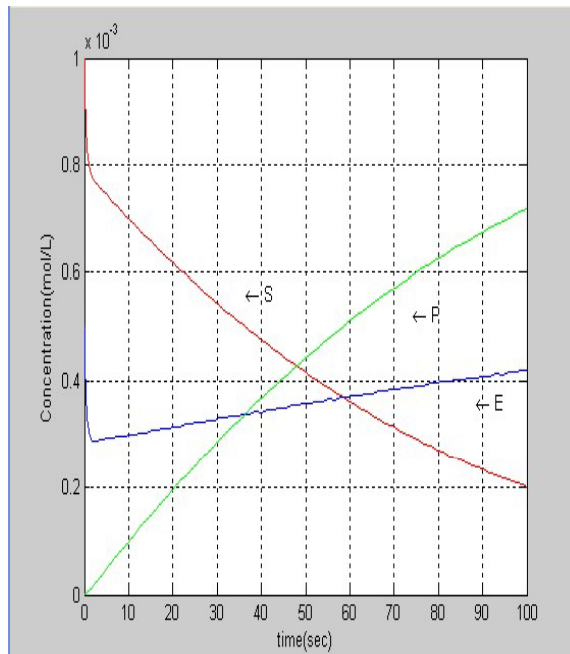


Parameter Variation

$k_2=0.5$



$k_2=0.05$



$k_2=0.005$

