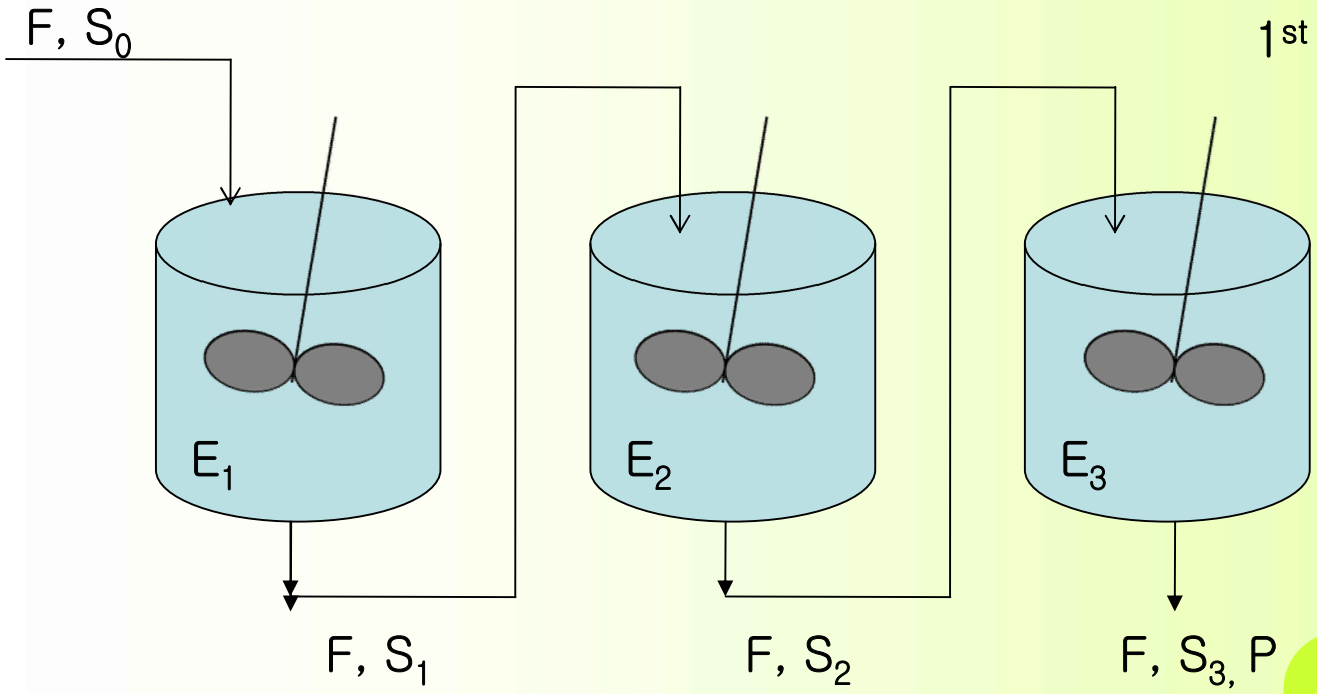
Reactor Cascade with Deactivating Enzyme

(DEACTENZ)

INTRODUCTION

The mass balance for the ith tank (i=1,2,3) $S -> P$



Tanks in series reactor with immobilized enzyme

INTRODUCTION

For the first tank

$$V_1 \frac{dS_1}{dt} = F(S_0 - S_1) + r_{S1} V_1$$

Dividing by V_1

$$\frac{dS_1}{dt} = \frac{(S_0 - S_1)}{\tau_1} + r_{S1}$$

INTRODUCTION

For the second and third tanks

$$\frac{dS_2}{dt} = \frac{(S_1 - S_2)}{\tau_2} + r_{S2}$$

$$\frac{dS_3}{dt} = \frac{(S_2 - S_3)}{\tau_3} + r_{S3}$$

$$V = V_1 = V_2 = V_3$$

$$\tau = \tau_1 = \tau_2 = \tau_3$$

The rate of substrate consumption

$$r_{Si} = -\frac{v_{\max} E_i S_i}{S_i + K_M + S_i^{\,2} / K_I}$$

INTRODUCTION

Enzyme (active)

$$V\frac{dE_i}{dt} = r_{Ei}V$$

The rate of enzyme deactivation

$$r_{Ei} = -k_D E_i$$

$$\frac{dE_i}{dt} = -k_D E_i$$

Product mass (kg)

$$P = \int_0^t F(S_0 - S_3)dt$$

NOMENCLATURE

Symbol	Description	Unit
E	Enzyme concentration	Kg/m^3
F	Flow rate	m^3/h
k_D	Deactivation constant	1/h
K_I	Inhibition constant	$Kmol/m^3$
K_M	Michaelis-Menten constant	$Kmol/m^3$
P	Total amount of product	Kmol
r_E	Reaction rate of deactivation	$Kg/(m^3\ h)$
r_S	Reaction rate of substrate	$Kmol/(m^3\ h)$
S	Substrate concentration	Mol/L
T	time	h
T_{LAG}	Time-on-stream difference	h
V_{max}	Maximum specific reaction rate	Kmol/kg h

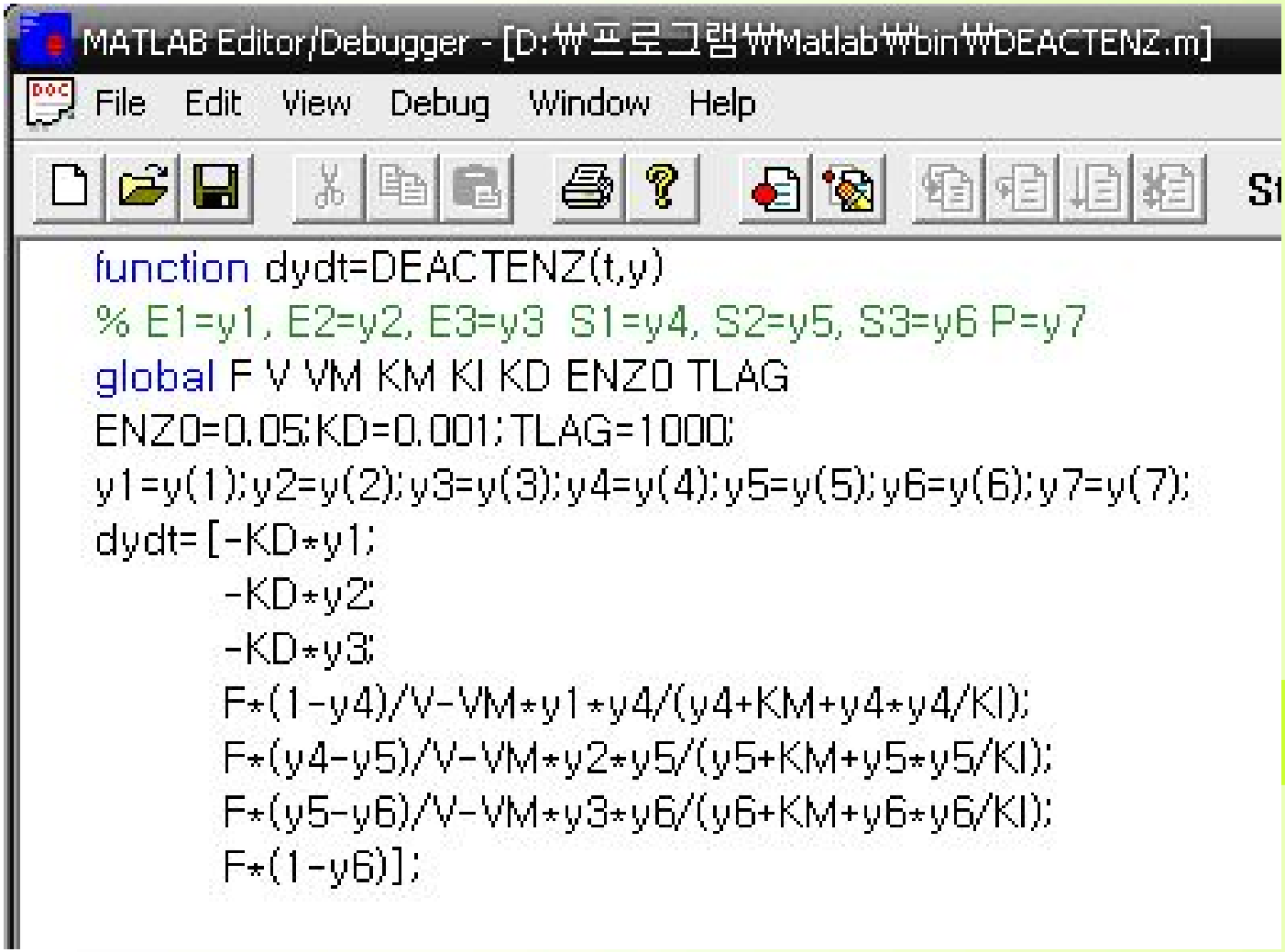
Matlab Program

MATLAB Command Window

File Edit Window Help

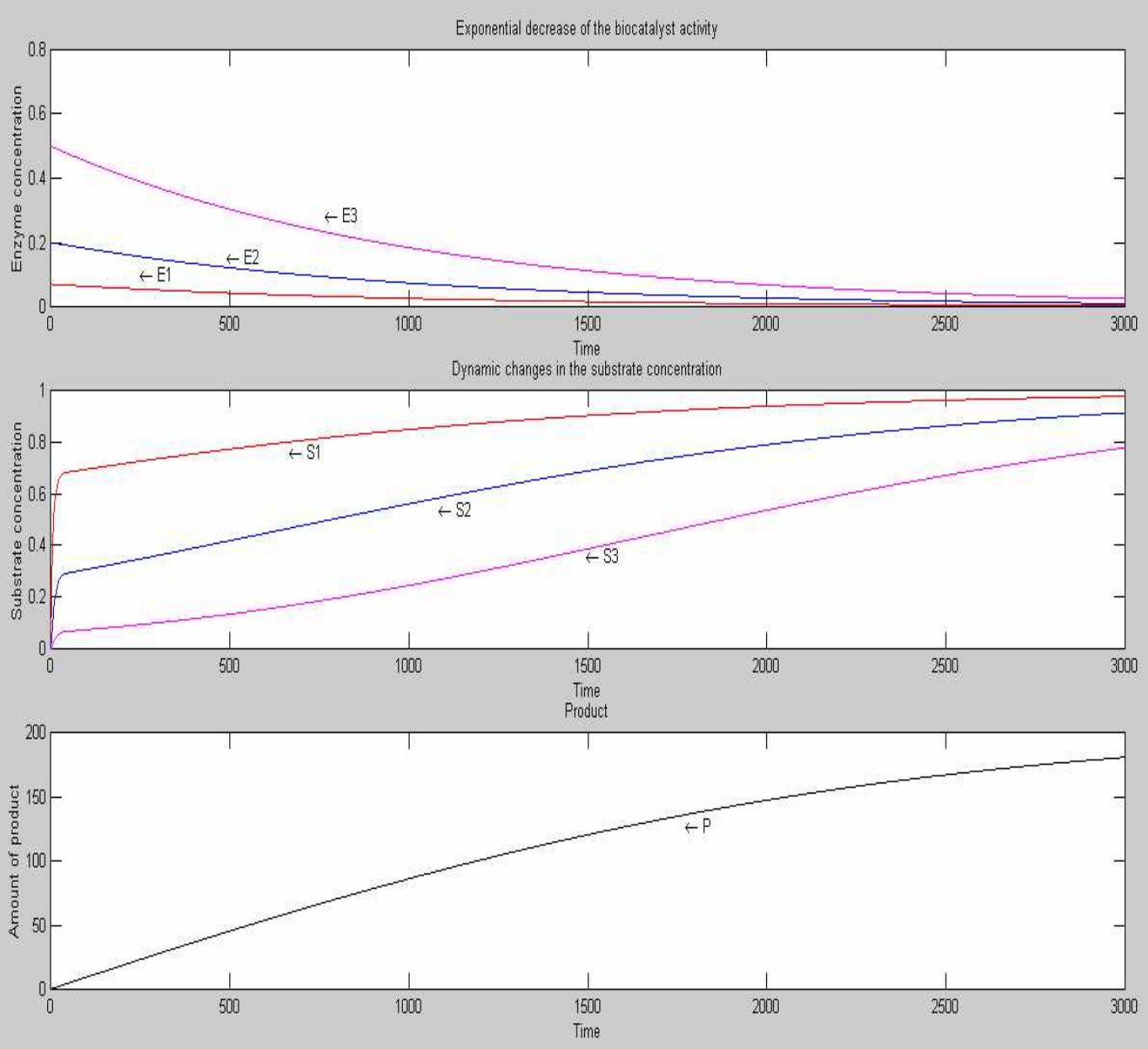
```
?global F V VM E0 E1 E2 E3 KM ENZ0 KI KD TLAG S0 SUB0
V=1;
F=0.1;
ENZ0=0.05;
TLAG=1000;
SUB0=140;
VM=42.98;                % Vmax
KM=61.59;                % Demensionless Michaelis constant
KI=6.85;                 % Demensionless Inhibition constant
KD=0.001;
S0=1;
y0=[0.07,0.2,0.5,0,0,0,0];                % 초기값
t0=0;
tf=3000;
[t,y]=ode45('DEACTENZ',t0:3:tf,y0);
E1=y(:,1);E2=y(:,2);E3=y(:,3);S1=y(:,4);S2=y(:,5);S3=y(:,6);P=y(:,7);
subplot(311),plot(t,E1,'r',t,E2,'b',t,E3,'m');
title('Exponential decrease of the biocatalyst activity');
xlabel('Time');ylabel('Enzyme concentration');
axis([0 3000 0 0.8]);
subplot(312),plot(t,S1,'r',t,S2,'b',t,S3,'m');
xlabel('Time');ylabel('Substrate concentration');
title('Dynamic changes in the substrate concentration');
axis([0 3000 0 1]);
subplot(313),plot(t,P,'k');
xlabel('Time');ylabel('Amount of product');
title('Product');
axis([0 3000 0 200]);
gtext('Wleftarrow E1');gtext('Wleftarrow E2');gtext('Wleftarrow E3');
gtext('Wleftarrow S1');gtext('Wleftarrow S2');gtext('Wleftarrow S3');
gtext('Wleftarrow P');
```

MODELING




```
function dydt=DEACTENZ(t,y)
% E1=y1, E2=y2, E3=y3  S1=y4, S2=y5, S3=y6 P=y7
global F V VM KM KI KD ENZ0 TLAG
ENZ0=0.05;KD=0.001;TLAG=1000;
y1=y(1);y2=y(2);y3=y(3);y4=y(4);y5=y(5);y6=y(6);y7=y(7);
dydt=[-KD*y1;
      -KD*y2;
      -KD*y3;
      F*(1-y4)/V-VM*y1*y4/(y4+KM+y4*y4/KI);
      F*(y4-y5)/V-VM*y2*y5/(y5+KM+y5*y5/KI);
      F*(y5-y6)/V-VM*y3*y6/(y6+KM+y6*y6/KI);
      F*(1-y6)];
```

RESULTS

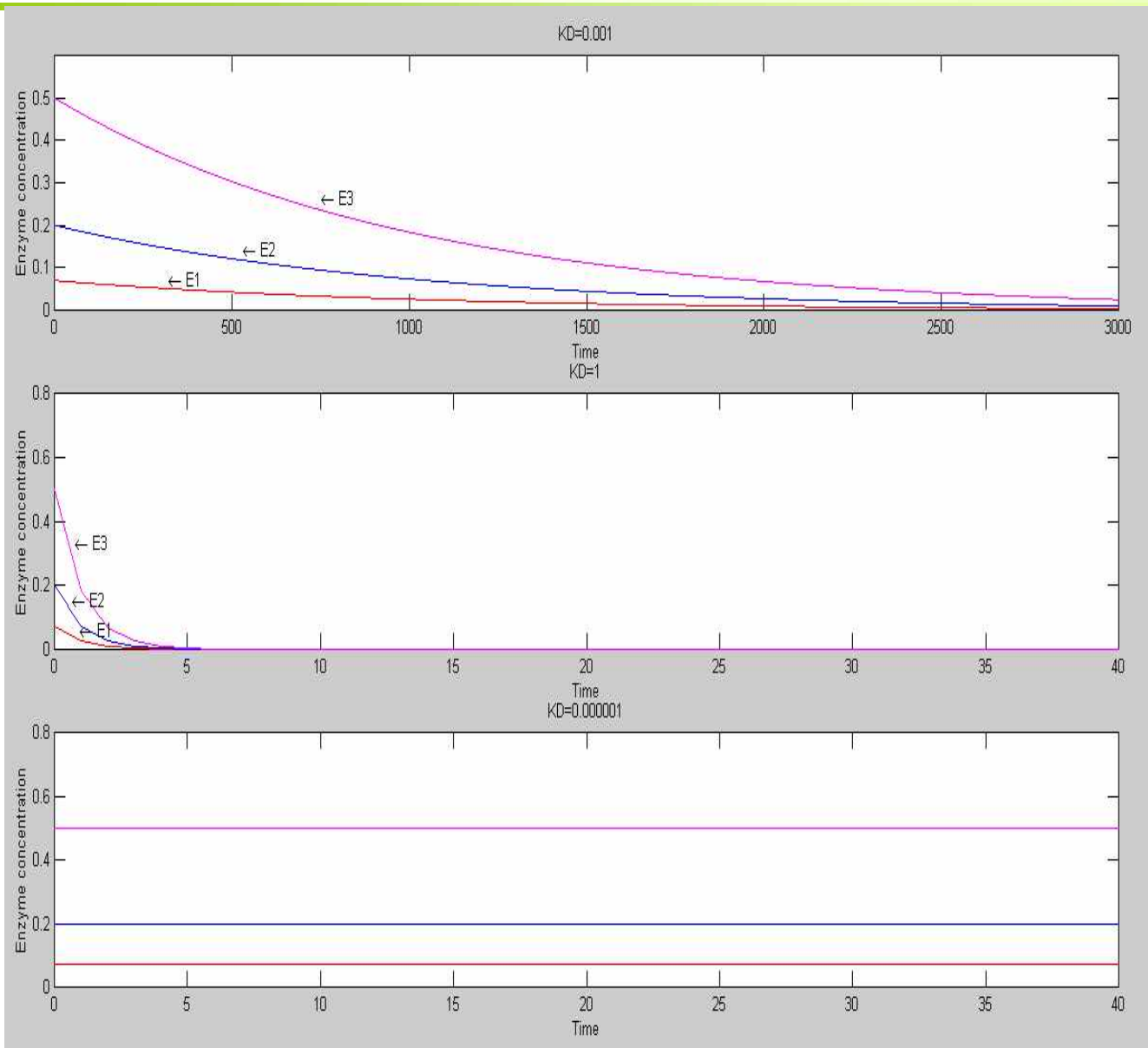


P1 : basic case

METHODS(Simulation cases)

	Basic case	P1
K_D=0.001	1	P2
	0.000001	P3
K_I=6.85	685	P4
	0.00685	P5
ENZ0=0.05	5	P6
	0.0005	P7

RESULTS

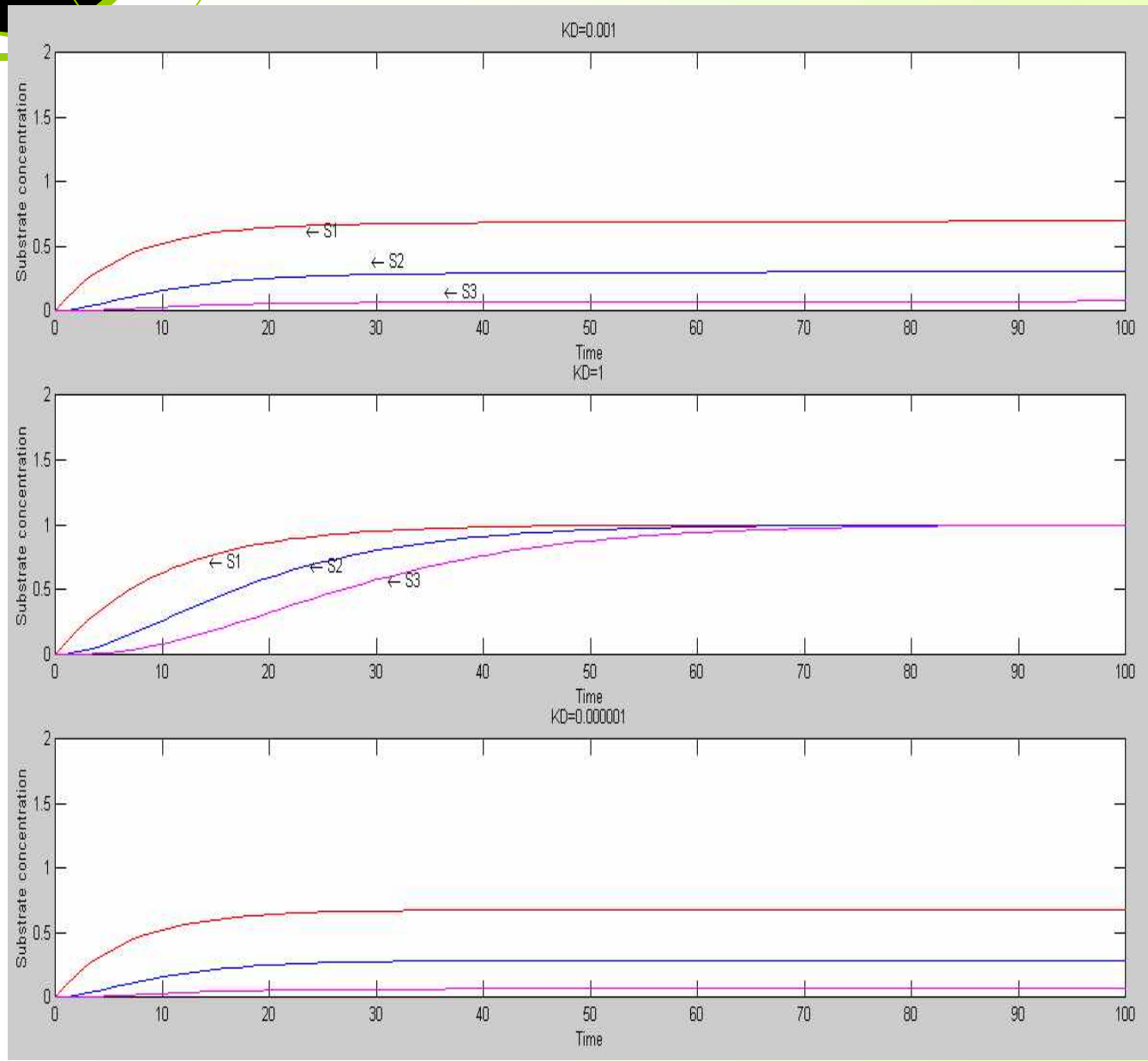


P1 : KD=0.001

P2 : KD=1

P3 : KD=0.000001

RESUL

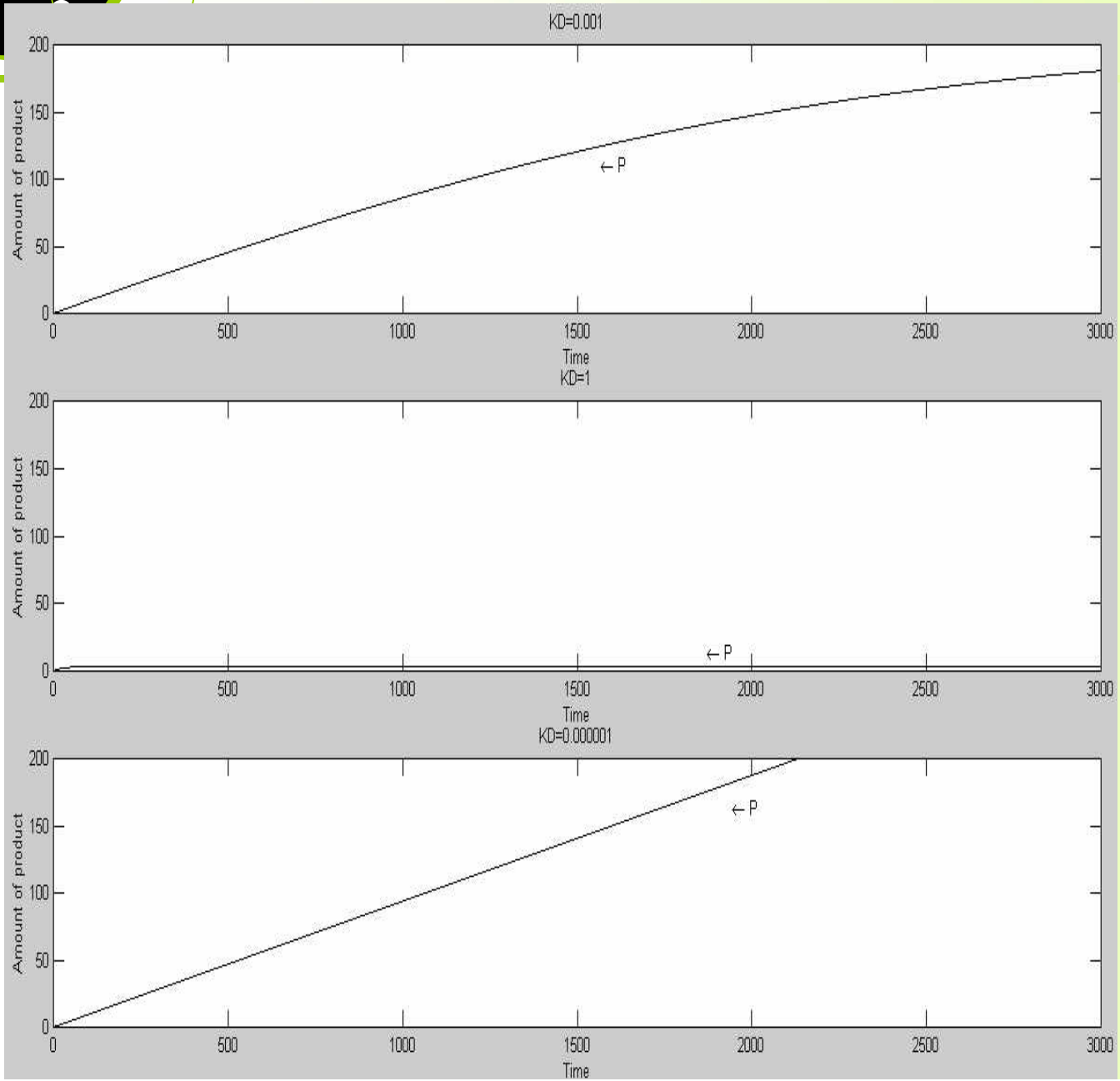


P1 : KD=0.001

P2 : KD=1

P3 : KD=0.000001

RESULTS

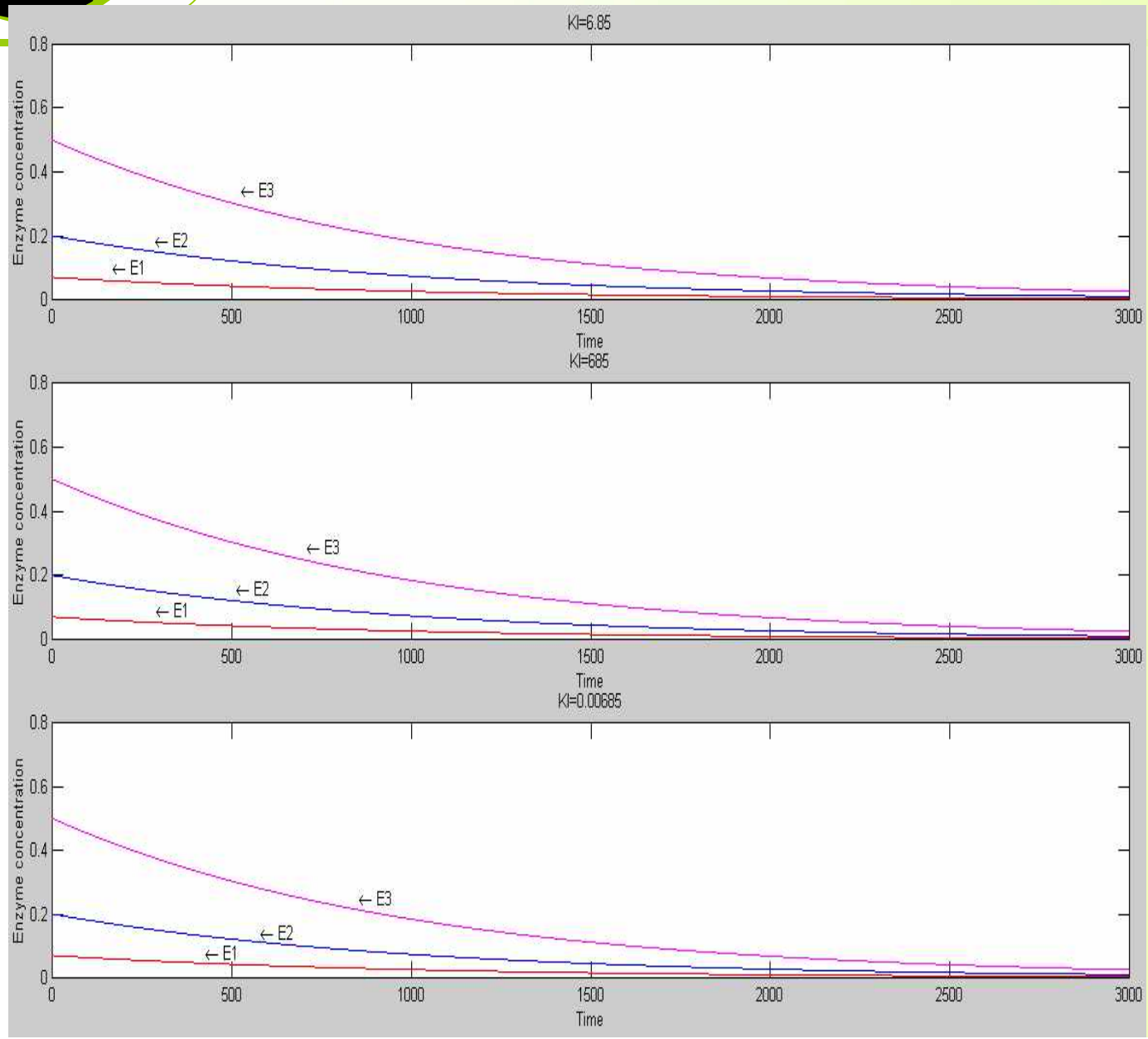


P1 : KD=0.001

P2 : KD=1

P3 : KD=0.000001

RESULTS

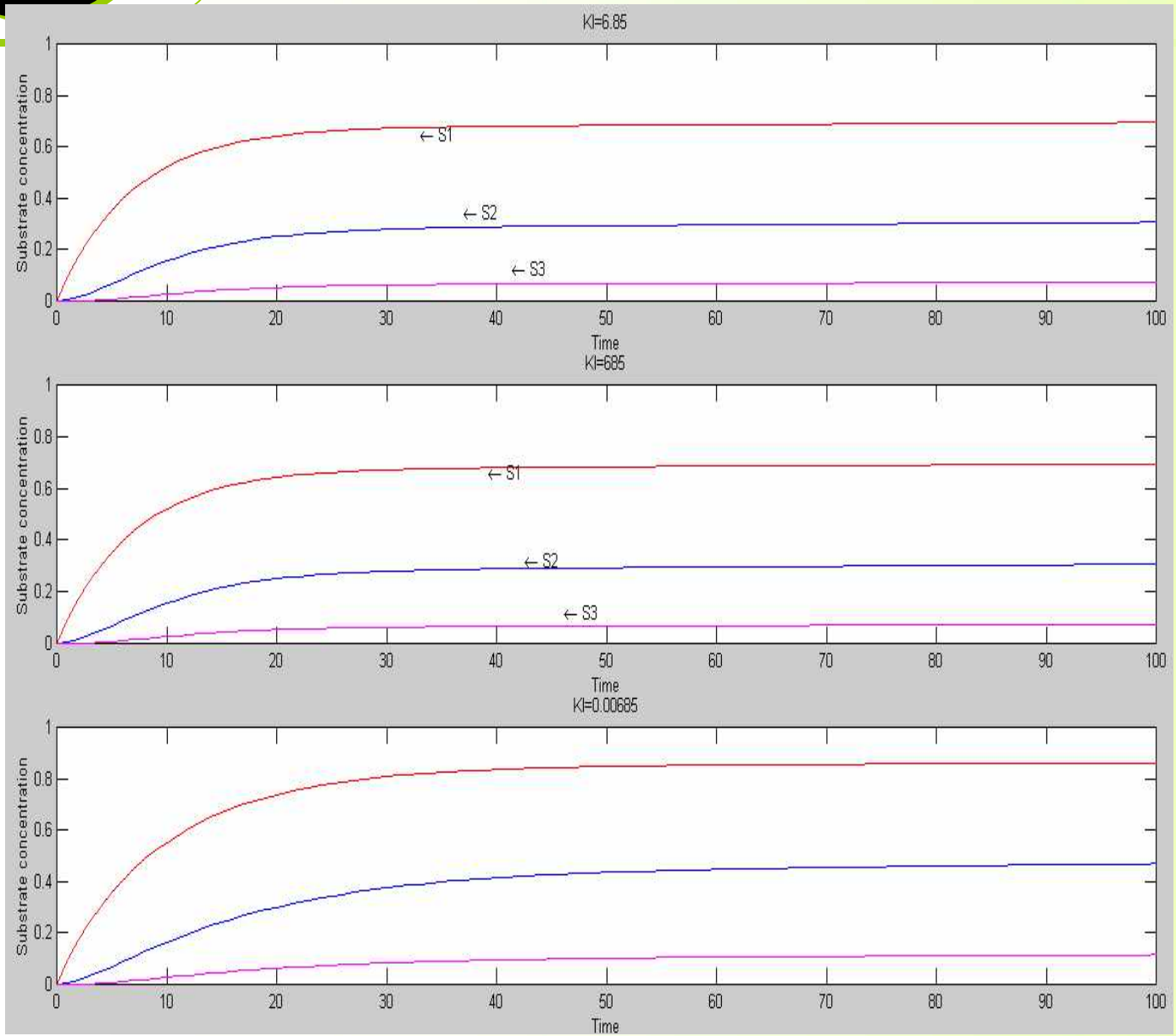


P1 : KI=6.85

P4 : KI=685

P5 : KI=0.00685

RESULTS

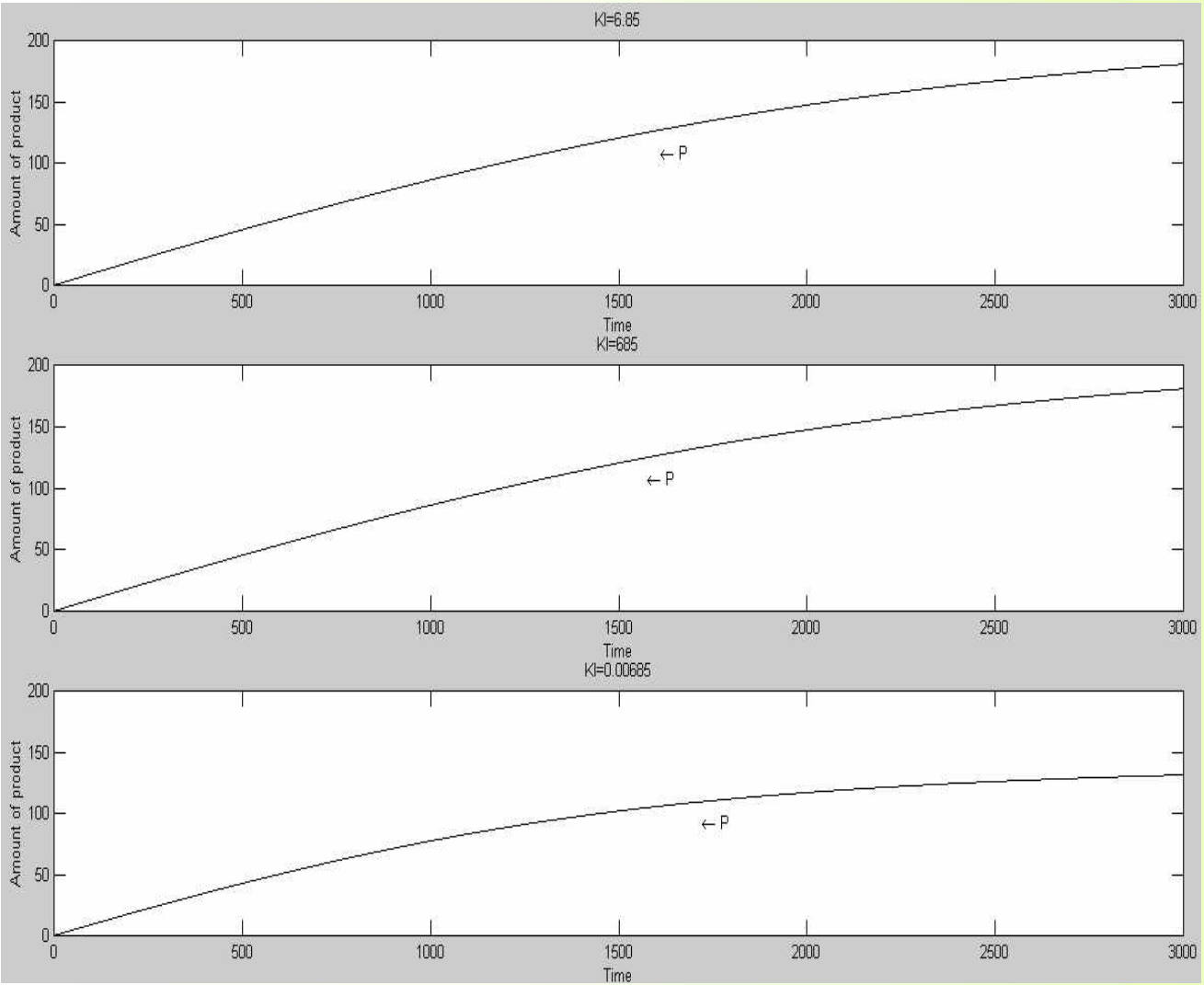


P1 : KI=6.85

P4 : KI=685

P5 : KI=0.00685

RESULTS

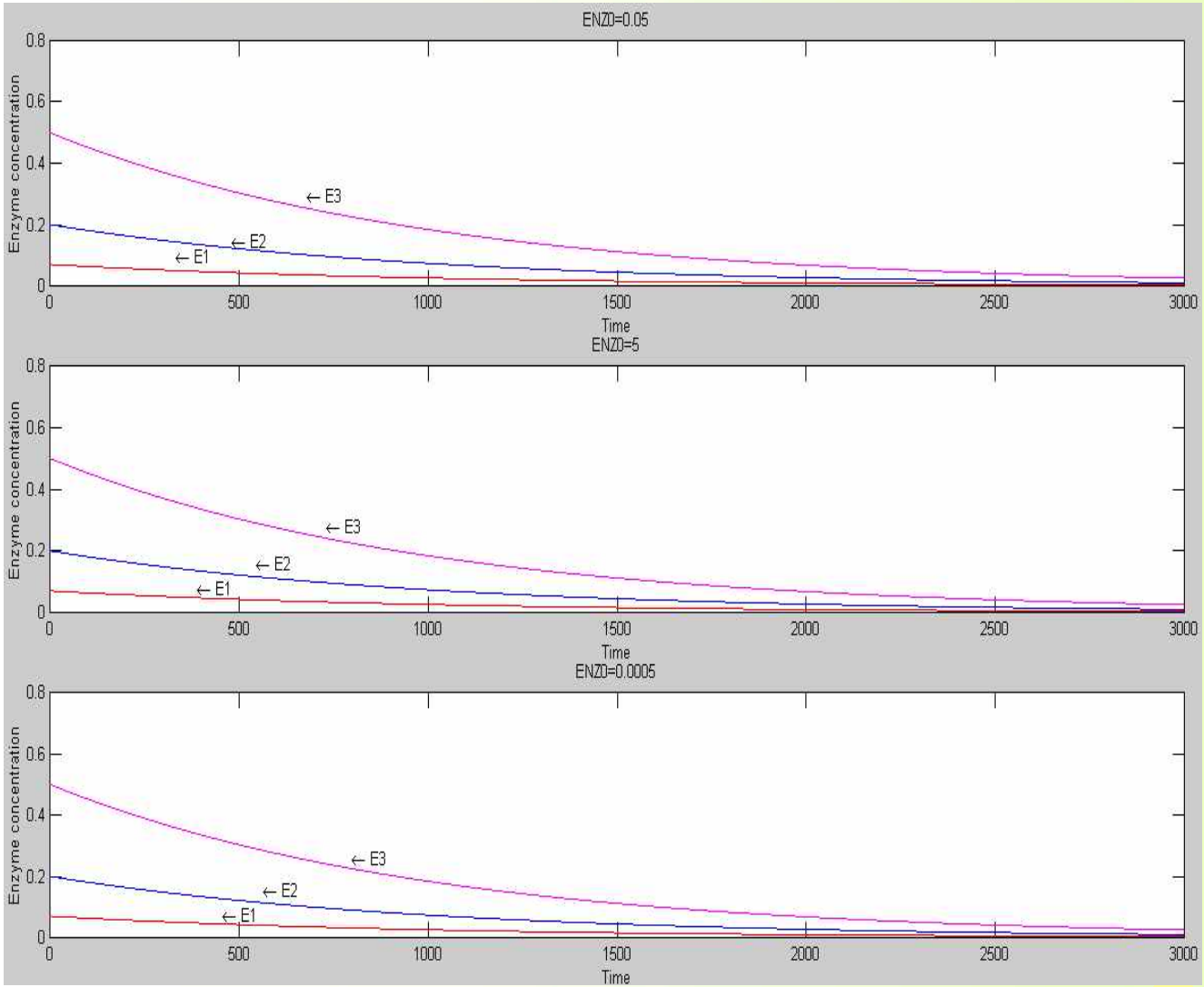


P1 : KI=6.85

P4 : KI=685

P5 : KI=0.00685

RESULTS

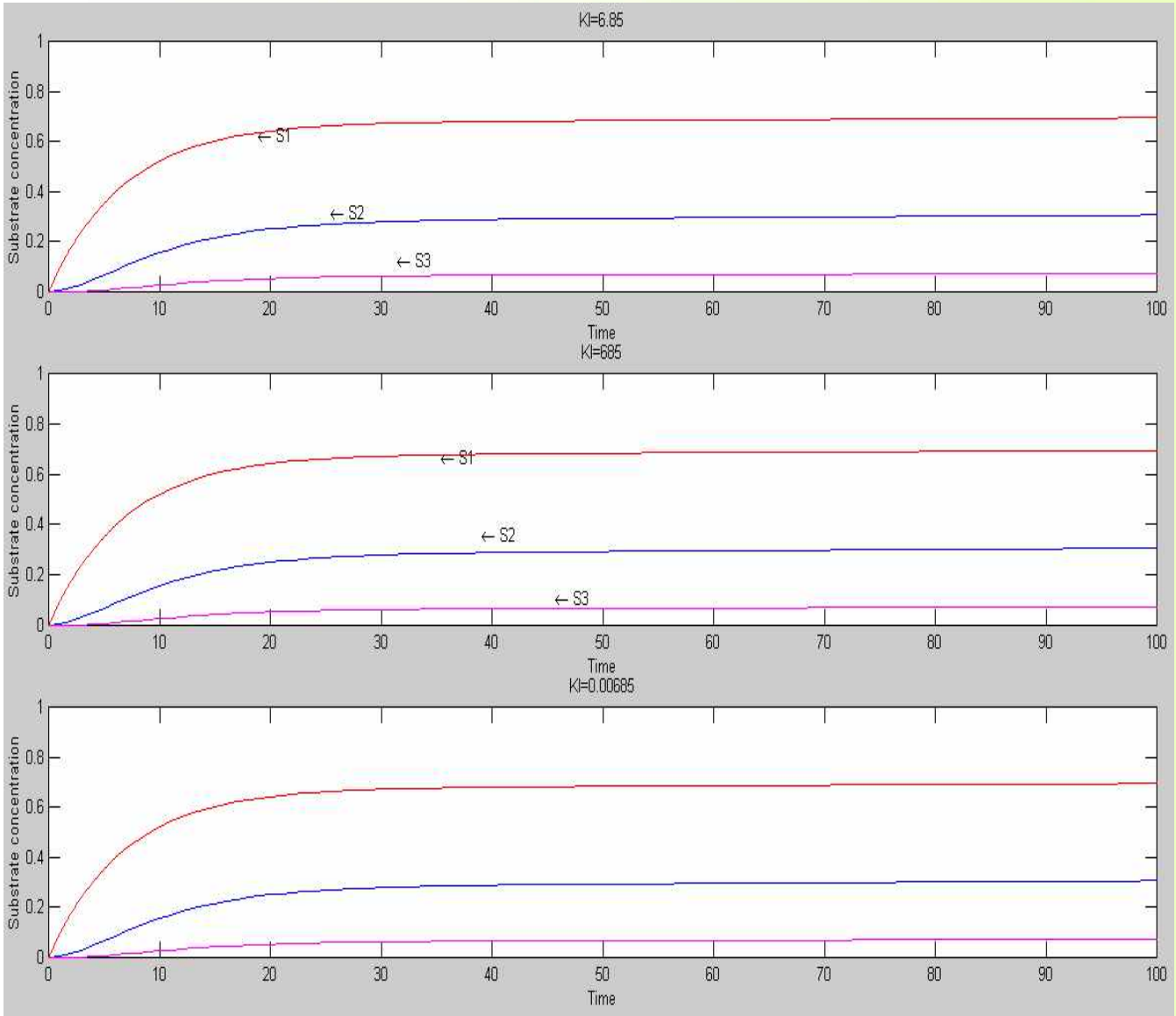


P1: ENZ0=0.05

P6 : ENZ0=5

P7 : ENZ0=0.005

RESULTS

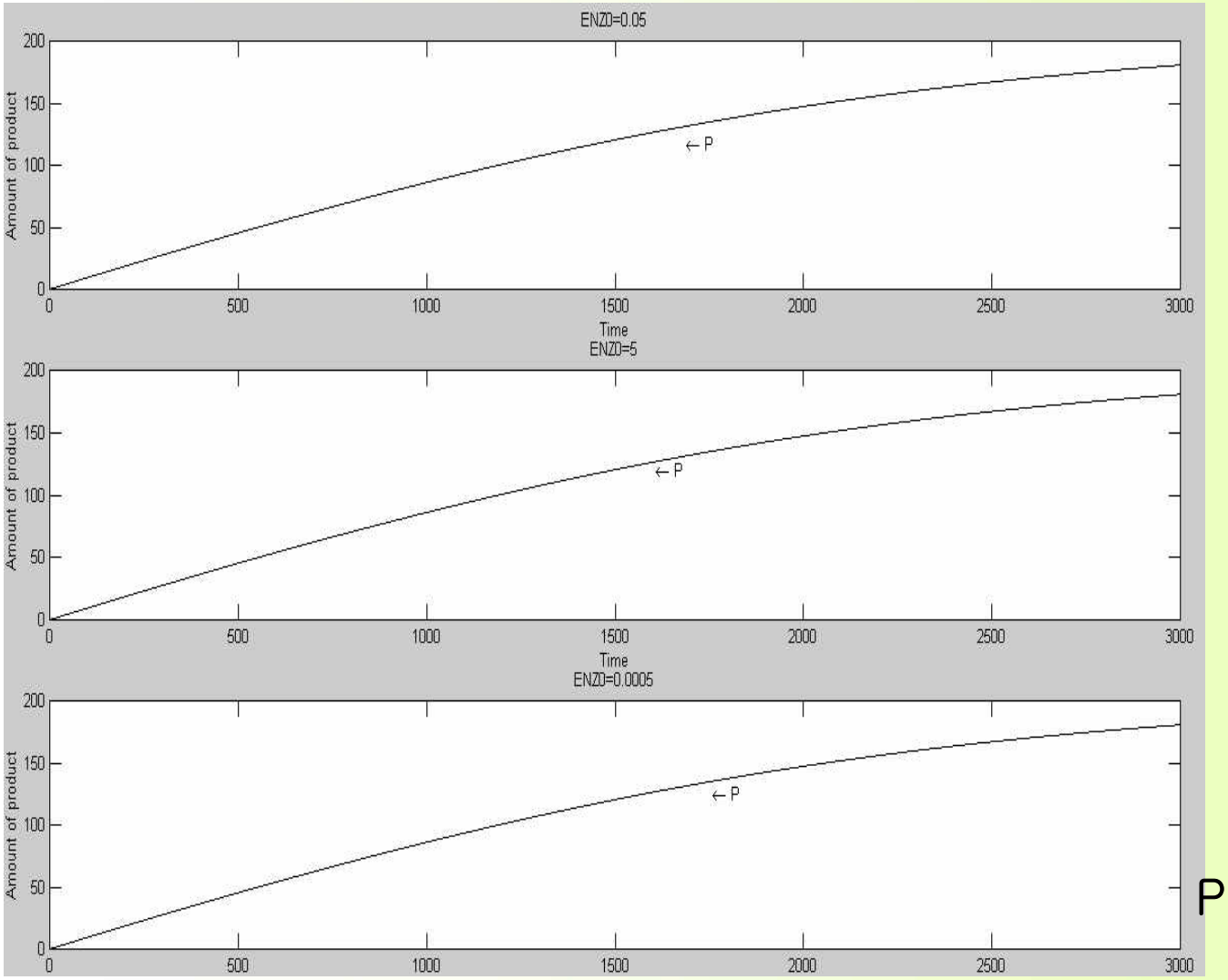


P1: ENZ0=0.05

P6 : ENZ0=5

P7 : ENZ0=0.005

RESULTS



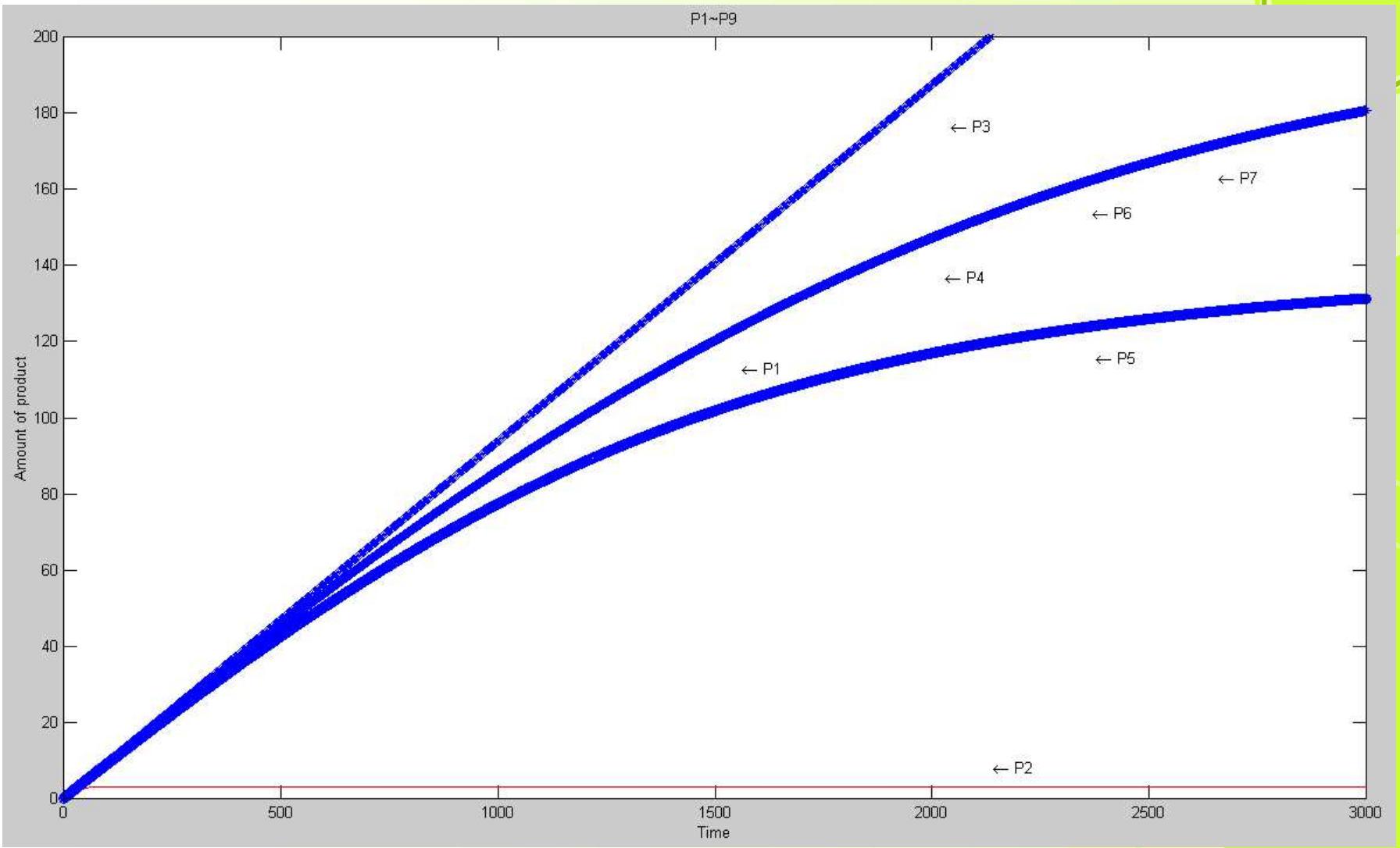
P1: ENZ0=0.05

P6 : ENZ0=5

P7 : ENZ0=0.005

RESULTS

P1 ~ P9



CONCLUSIONS

- Exponential decrease of the biocatalyst activity
- K_D (Deactivation constant) ↓ : productivity ↑
- K_I (Inhibition constant) ↓ : productivity ↓