

1.

a. solve y^* as a fun of $[L]$ at s.s

at s.s. $\frac{d[R^*]}{dt} = \frac{d[X^*]}{dt} = \frac{d[Y^*]}{dt} = 0$

$$\frac{\delta_1}{V_2} [R_T] = 5$$

$$\frac{\delta_3}{V_4} [X_T] = 10$$

$$(1) k_{on}[R][L] - k_{off}[R^*] = 0$$

$$(2) \frac{v_1 [X]}{k_1 + [X]} - \frac{v_2 [X^*]}{k_2 + [X^*]} = 0; v_1 = \delta_1 [R^*]$$

$$(3) \frac{v_3 [Y]}{k_3 + [Y]} - \frac{v_4 [Y^*]}{k_4 + [Y^*]} = 0; v_3 = \delta_3 [X^*]$$

Non dimensionalize:

$$x^* = \frac{[X^*]}{X_T}; k_1 = \frac{k_1}{X_T}; k_2 = \frac{k_2}{X_T}; k_3 = \frac{k_3}{Y_T}; k_4 = \frac{k_4}{Y_T}; k_D = \frac{k_{off}}{(k_{on}[L])}$$

$$\theta_B = \frac{[R^*]}{R_T}; \frac{v_1}{V_2} = \left(\frac{\delta_1 \theta_B}{V_2}\right) R_T; \frac{v_3}{V_4} = \left(\frac{\delta_3 X^*}{V_4}\right) X_T$$

(1)

$$\frac{k_{off}}{k_D} (R_T - [R^*]) - k_{off}[R^*] = 0$$

$$\frac{1}{k_D} (R_T - [R^*]) - [R^*] = 0$$

$$\frac{1}{k_D} (R_T - R_T \theta_B) - \theta_B R_T = 0$$

$$\frac{1}{k_D} = \frac{\theta_B}{(1 - \theta_B)}$$

or $\theta_B = \frac{1}{1 + k_D}$

(3)

$$\frac{\frac{V_3}{V_4} (Y_T - [Y^*])}{X_3 Y_T + (Y_T - [Y^*])} - \frac{[Y^*]}{k_4 Y_T + [Y^*]} = 0$$

$$\frac{\frac{V_3}{V_4} (Y_T - y^* Y_T)}{X_3 Y_T + (Y_T - y^* Y_T)} - \frac{y^* Y_T}{k_4 Y_T + y^* Y_T} = 0$$

$$\frac{\frac{V_3}{V_4} (1 - y^*)}{k_3 + (1 - y^*)} - \frac{y^*}{k_4 + y^*} = 0$$

Simplify:

$$\frac{(1 - \frac{V_3}{V_4}) y^{*2}}{a} + \frac{(\frac{V_3}{V_4} - \frac{V_3}{V_4} k_4 - k_3 - 1) y^* + \frac{V_3}{V_4} k_4}{b} = 0$$

$$y^* = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

$x = 0$

(2)

$$\frac{\delta_1 [R^*] (X_T - [X^*])}{X_1 X_T + (X_T - [X^*])} = \frac{v_2 [X^*]}{k_2 X_T + [X^*]}$$

$$\left(\frac{\delta_1 \theta_B}{V_2}\right) R_T (X_T - [X^*]) (k_2 X_T + [X^*]) = [X^*] (k_1 X_T + X_T - [X^*])$$

$$\left(\frac{\delta_1 \theta_B}{V_2}\right) R_T (X_T - X^* X_T) (k_2 X_T + X^* X_T) = X^* X_T (k_1 X_T + X_T - X^* X_T)$$

$$\left(\frac{\delta_1 \theta_B}{V_2}\right) R_T (1 - X^*) (k_2 + X^*) = X^* (X_1 + 1 - X^*)$$

$$\frac{(1 - \frac{V_1}{V_2}) X^{*2}}{a} + \frac{(\frac{V_1}{V_2} - \frac{V_1}{V_2} k_2 - k_1 - 1) X^* + \frac{V_1}{V_2} k_2}{b} = 0$$

$$y^* = \frac{(1 + k_3 + \frac{V_1}{V_4} k_4 - \frac{V_1}{V_4}) \pm \sqrt{(\frac{V_1}{V_4} - \frac{V_1}{V_4} k_4 - k_3 - 1)^2 - 4(1 - \frac{V_1}{V_4})(\frac{V_1}{V_4} k_2)}}{2(1 - \frac{V_1}{V_4})}$$

where $\frac{V_3}{V_4} = \frac{\delta_3 X^*}{V_4} X_T$

$$x^* = \frac{(\frac{V_1}{V_2} k_2 + k_1 + 1 - \frac{V_1}{V_2}) \pm \sqrt{(\frac{V_1}{V_2} - \frac{V_1}{V_2} k_2 - k_1 - 1)^2 - 4(1 - \frac{V_1}{V_2})(\frac{V_1}{V_2} k_2)}}{2(1 - \frac{V_1}{V_2})}$$

where $\frac{v_1}{V_2} = \frac{\delta_1 \theta_B}{V_2} R_T$

1 b) $K_1 = K_2 = K_3 = K_4 = K$, $K = 0.1 \text{ \& } K = 10$ plot θ_B , x^* and y^* v.s $\frac{1}{\theta_B}$. Given $\frac{r_1}{V_2} [K_T] = 5$

$$x^* = \frac{\left(\frac{V_1}{V_2} K + K + 1 - \frac{V_1}{V_2}\right) \pm \left[\left(\frac{V_1}{V_2} - \frac{V_1}{V_2} K - K - 1\right)^2 - 4\left(1 - \frac{V_1}{V_2}\right)\left(\frac{V_1}{V_2} K\right)\right]^{1/2}}{2\left(1 - \frac{V_1}{V_2}\right)}$$

$$\frac{K_3}{V_4} [K_T] = 10$$

$$= \frac{\left(5\theta_B K + K + 1 - 5\theta_B\right) \pm \left[\left(5\theta_B - 5\theta_B K - K - 1\right)^2 - 4\left(1 - 5\theta_B\right)\left(5\theta_B K\right)\right]^{1/2}}{2\left(1 - 5\theta_B\right)}$$

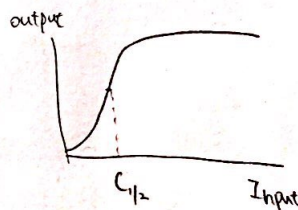
$$\frac{1}{V_2} = \frac{\delta_1 \theta_B}{V_2} R_T = 5 \cdot \theta_B$$

$$y^* = \frac{\left(1 + K + 10x^* K - 10x^*\right) \pm \left[\left(10x^* - 10x^* K - K - 1\right)^2 - 4\left(1 - 10x^*\right)\left(10x^* K\right)\right]^{1/2}}{2\left(1 - 10x^*\right)}$$

$$\frac{V_3}{V_4} = \frac{\delta_3 x^*}{V_4} X_T = 10x^*$$

(plot should in matlab.)

c). Hill coeff $\text{Output} = \frac{\text{Input}^{n_H}}{C_{1/2}^{n_H} + \text{Input}^{n_H}}$



Using Excel Regression fitting. get.

$K = 0.1$

$$\text{output} = \frac{m \cdot \text{Input}^{n_H}}{C_{1/2}^{n_H} + \text{Input}^{n_H}}$$

3rd parameter (if necessary)

$\frac{1}{K_D}$ vs. θ_B : $n = 1$; $C_{1/2} = 2.22$ $m = 1.11$

$\frac{1}{K_D}$ vs x^* : $n = 3.35$; $C_{1/2} = 0.483$ $m = 0.975$

$\frac{1}{K_D}$ vs y^* : $n = 7.08$; $C_{1/2} = 0.245$ $m = 0.992$

$K = 10$

$\frac{1}{K_D}$ vs. θ_B : $n = 1.00$ $C_{1/2} = 1.00$

$\frac{1}{K_D}$ vs x^* : $n = 1.03$ $C_{1/2} = 0.174$ $m = 0.843$

$\frac{1}{K_D}$ vs. y^* : $n = 1.057$ $C_{1/2} = 0.0200$ $m = 0.900$

d). changes calculated from matlab.

e). See answer in matlab.

$K = 0.1$ $\theta_B: 43.48\%$, $x^*: 101.83\%$, $y^*: 402.58\%$

$K = 10$ $\theta_B: 43.48\%$, $x^*: 27.97\%$, $y^*: 5.66\%$

$$V_{max1} = V_{max2} = 5 \quad V_{max3} = V_{max4} = 1 \quad K_{S1} = K_{S2} = K_{S3} = K_{S4} = 5.0 \quad K_{I1} = K_{I2} = 1.$$

$S_{tot} = 100$ Find S.S of [A], [B], [C] in absence of inhibitors.

S.S. $\frac{d[B]}{dt} = \frac{d[C]}{dt} = 0$. No inhibitor, $[I_1] = 0 = [I_2]$.

$$① V_1 - V_2 = 0$$

$$② V_2 - V_3 = 0 \Rightarrow$$

$$① \frac{V_{max1}[A]}{\left(1 + \frac{[I_1]}{K_{I1}}\right)(K_{S1} + [A])} - \frac{V_{max3}[B]}{K_{S3} + [B]} = 0$$

$$\frac{V_{max1}[A]}{K_{S1} + [A]} - \frac{V_{max3}[B]}{K_{S3} + [B]} = 0$$

$$\frac{5[A]}{5 + [A]} - \frac{[B]}{5 + [B]} = 0$$

$$② \frac{V_{max2}[A]}{\left(1 + \frac{[I_2]}{K_{I2}}\right)(K_{S2} + [A])} - \frac{V_{max4}[C]}{K_{S4} + [C]} = 0$$

$$\frac{5[A]}{5 + [A]} - \frac{[C]}{5 + [C]} = 0$$

$$③ [A] = S_{tot} - [B] - [C] = 100 - [B] - [C]$$

Solve ① ② ③ get $[A] = 1.1097$

$$[B] = 49.4451$$

$$[C] = 49.4451$$

b). Inhibitor:

$$① \frac{5[A]}{\left(1 + \frac{[I_1]}{K_{I1}}\right)(5 + [A])} - \frac{[B]}{5 + [B]} = 0$$

$$② \frac{5[A]}{\left(1 + \frac{[I_2]}{K_{I2}}\right)(5 + [A])} - \frac{[C]}{5 + [C]} = 0$$

Table of Contents

ChemE 7770 PS4	1
Problem 1	1
1a)	1
1b).	1
1c)	3
1d)	3
e). Importance of parameter tuning	4
Problem #2	5
2a)	5
2b)	5
2c)	6
2d)	6
2e)	7

ChemE 7770 PS4

```
clear all; close all; clc;
```

Problem 1

1a)

See the attached paper for calculation steps.

1b).

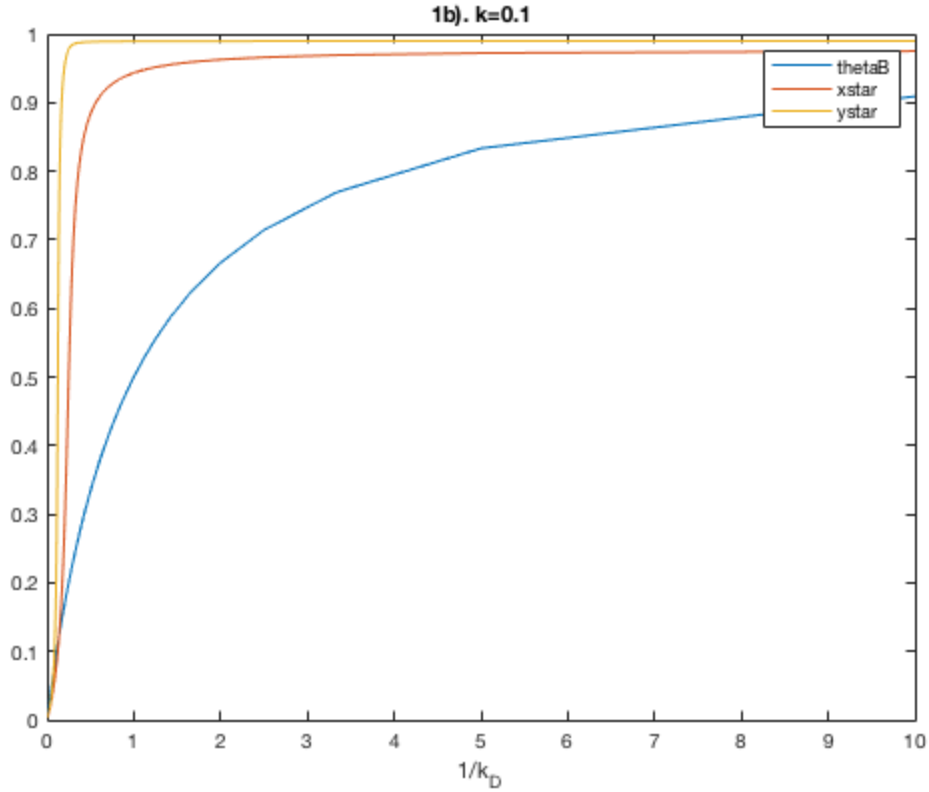
```
global k_D k [result,fval,exit,output]=fsolve(@Signaling,A0,options); k=0.1;

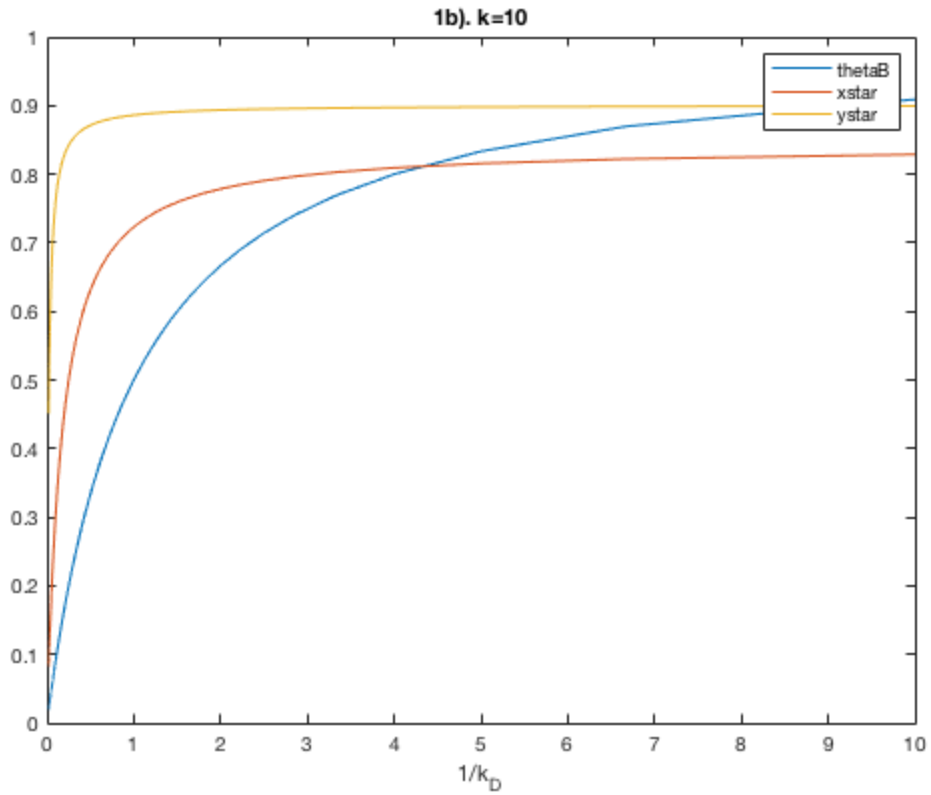
k_D=0.1;k1=0.1;
for i=1:1000
    thetaB(i)=1/(1+k_D(i));
    xstar(i)=((5.*thetaB(i).*k1+k1+1-5.*thetaB(i))-
    ((5.*thetaB(i)-5.*thetaB(i).*k1-
    k1-1).^2-4.*(1-5.*thetaB(i)).*(5.*thetaB(i).*k1)).^(0.5))./
    (2.*(1-5.*thetaB(i))));
    ystar(i)=((1+k1+10.*xstar(i).*k1-10.*xstar(i))-
    ((10.*xstar(i)-10.*xstar(i).*k1-
    k1-1).^2-4.*(1-10.*xstar(i)).*(10.*xstar(i).*k1)).^(0.5))./
    (2.*(1-10.*xstar(i))));
    k_D(i+1)=k_D(i)+0.1;
end
kd=k_D(1:length(k_D)-1);
figure (1)
plot(1./kd,thetaB,1./kd,xstar,1./kd,ystar);
legend('thetaB','xstar','ystar');
```

```

xlabel('1/k_D');
title('1b). k=0.1');
% k=10
k2=10;
k_D=0.1;
for i=1:1000
    thetaB2(i)=1/(1+k_D(i));
    xstar2(i)=((5.*thetaB2(i).*k2+k2+1-5.*thetaB2(i))-
    ((5.*thetaB2(i)-5.*thetaB2(i).*k2-
    k2-1).^2-4.*(1-5.*thetaB2(i)).*(5.*thetaB2(i).*k2)).^(0.5))./
    (2.*(1-5.*thetaB2(i))));
    ystar2(i)=((1+k2+10.*xstar2(i).*k2-10.*xstar2(i))-
    ((10.*xstar2(i)-10.*xstar2(i).*k2-
    k2-1).^2-4.*(1-10.*xstar2(i)).*(10.*xstar2(i).*k2)).^(0.5))./
    (2.*(1-10.*xstar2(i))));
    k_D(i+1)=k_D(i)+0.05;
end
kd=k_D(1:length(k_D)-1);
xstar2(79)=0.5;
ystar2(79)=0.842;
figure (2)
plot(1./kd,thetaB2,1./kd,xstar2,1./kd,ystar2);
legend('thetaB','xstar','ystar');
xlabel('1/k_D');
title('1b). k=10');

```





1c)

Hill Coeff See excel for detail. Hill coeff for $1/k_D$ vs θ_B , x_{star} , y_{star} respectively: for $k=0.1$, $n=1$ 3.35 7.08; $c1/2=2.22$ 0.483 0.245; for $k=10$, $n=1$ 1.03 1.057; $c1/2=1$ 0.174 0.02

1d)

Change as k_D changes $k=0.1$;

```
KD=1/0.1; k1=0.1;
thetaB1d=1/(1+KD);
xstar1d=((5.*thetaB1d.*k1+k1+1-5.*thetaB1d)-
((5.*thetaB1d-5.*thetaB1d.*k1-
k1-1).^2-4.*(1-5.*thetaB1d).*(5.*thetaB1d.*k1)).^(0.5))./
(2.*(1-5.*thetaB1d)));
ystar1d=((1+k1+10.*xstar1d.*k1-10.*xstar1d)-
((10.*xstar1d-10.*xstar1d.*k1-
k1-1).^2-4.*(1-10.*xstar1d).*(10.*xstar1d.*k1)).^(0.5))./
(2.*(1-10.*xstar1d)));
KD2=1/0.15;
thetaB1d2=1/(1+KD2);
xstar1d2=((5.*thetaB1d2.*k1+k1+1-5.*thetaB1d2)-
((5.*thetaB1d2-5.*thetaB1d2.*k1-
k1-1).^2-4.*(1-5.*thetaB1d2).*(5.*thetaB1d2.*k1)).^(0.5))./
(2.*(1-5.*thetaB1d2)));
```

```

ystar1d2=((1+k1+10.*xstar1d2.*k1-10.*xstar1d2)-
((10.*xstar1d2-10.*xstar1d2.*k1-
k1-1).^2-4.*(1-10.*xstar1d2).*(10.*xstar1d2.*k1)).^(0.5))./
(2.*(1-10.*xstar1d2)));
thetaB_ch=abs((thetaB1d-thetaB1d2)./thetaB1d).*100;
xstar_ch=abs((xstar1d-xstar1d2)./xstar1d).*100;
ystar_ch=abs((ystar1d-ystar1d2)./ystar1d).*100;
disp(['% change of thetaB, xstar, and ystar for k=0.1
respectively: ',num2str(thetaB_ch), '%, ',num2str(xstar_ch), '%, and
',num2str(ystar_ch), '%']);

% k=10;
KD=1/0.1; k2=10;
thetaB1d=1/(1+KD);
xstar1d=((5.*thetaB1d.*k2+k2+1-5.*thetaB1d)-
((5.*thetaB1d-5.*thetaB1d.*k2-
k2-1).^2-4.*(1-5.*thetaB1d).*(5.*thetaB1d.*k2)).^(0.5))./
(2.*(1-5.*thetaB1d)));
ystar1d=((1+k2+10.*xstar1d.*k2-10.*xstar1d)-
((10.*xstar1d-10.*xstar1d.*k2-
k2-1).^2-4.*(1-10.*xstar1d).*(10.*xstar1d.*k2)).^(0.5))./
(2.*(1-10.*xstar1d)));
KD2=1/0.15;
thetaB1d2=1/(1+KD2);
xstar1d2=((5.*thetaB1d2.*k2+k2+1-5.*thetaB1d2)-
((5.*thetaB1d2-5.*thetaB1d2.*k2-
k2-1).^2-4.*(1-5.*thetaB1d2).*(5.*thetaB1d2.*k2)).^(0.5))./
(2.*(1-5.*thetaB1d2)));
ystar1d2=((1+k2+10.*xstar1d2.*k2-10.*xstar1d2)-
((10.*xstar1d2-10.*xstar1d2.*k2-
k2-1).^2-4.*(1-10.*xstar1d2).*(10.*xstar1d2.*k2)).^(0.5))./
(2.*(1-10.*xstar1d2)));
thetaB_ch2=abs((thetaB1d-thetaB1d2)./thetaB1d).*100;
xstar_ch2=abs((xstar1d-xstar1d2)./xstar1d).*100;
ystar_ch2=abs((ystar1d-ystar1d2)./ystar1d).*100;
disp(['% change of thetaB, xstar, and ystar for k=10 respectively:
',num2str(thetaB_ch2), '%, ',num2str(xstar_ch2), '%, and
',num2str(ystar_ch2), '%']);

% change of thetaB, xstar, and ystar for k=0.1 respectively: 43.4783%,
101.8261%, and 402.5798%
% change of thetaB, xstar, and ystar for k=10 respectively: 43.4783%,
27.9659%, and 5.6566%

```

e). Importance of parameter tuning

The output of xstar and ystar has big changes as input has a small changes for k=0.1 while for k=10 the change is less. Thus, it's important to define parameter that fits the model. In this case, if we want the output to be very sensitive, we want k=0.1, on the other hand, if we want the output to has less variation as input varies, we would want k=10.

Problem #2

2a)

```
B0=[4 4 6]';  
[Soln,fval,exit,output]=fsolve(@NoInhi,B0);  
display(Soln);
```

Equation solved.

fsolve completed because the vector of function values is near zero as measured by the value of the function tolerance, and the problem appears regular as measured by the gradient.

Soln =

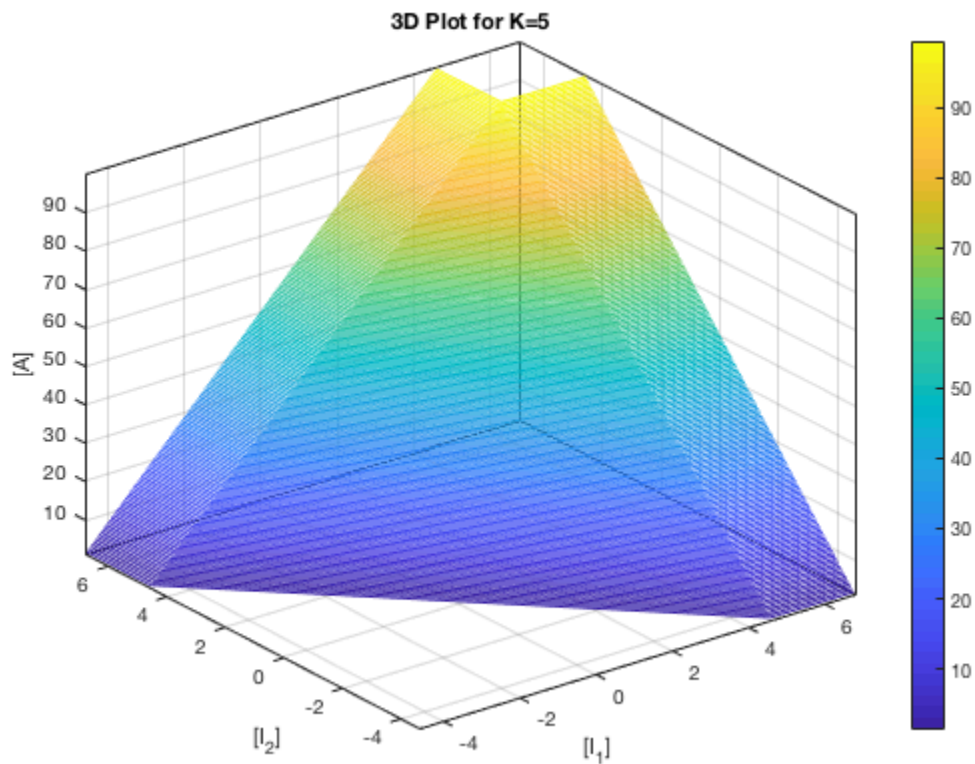
```
1.1097  
49.4451  
49.4451
```

2b)

```
I_1=0.01:100:1000;  
I_2=0.01:100:1000;  
points=length(I_1);  
Aconc=zeros(length(I_1),length(I_2));  
for j=1:points  
    for i=1:points  
        syms A I1 I2  
        I1=I_1(j);  
        I2=I_2(i);  
        eqn=A.*(1+25./((1+I1).*(5+A)-5.*A))+25./((1+I2).*(5+A)-5.*A))==100;  
        sol=solve(eqn,A);  
        sol=double(sol);  
        sol=sol(sol>=0);  
        [m,n]=(size(sol));  
        if m>1  
            val=min(sol);  
        else  
            val=sol;  
        end  
        Aconc(j,i)=val;  
    end  
end  
figure (4)  
contour3(log(I_1),log(I_2),Aconc,200);  
colorbar  
title('3D Plot for K=5');  
xlabel('I_1');
```



```
ylabel('I_2');
xlabel('I_1');
```



2c)

The system is a OR logic gate.

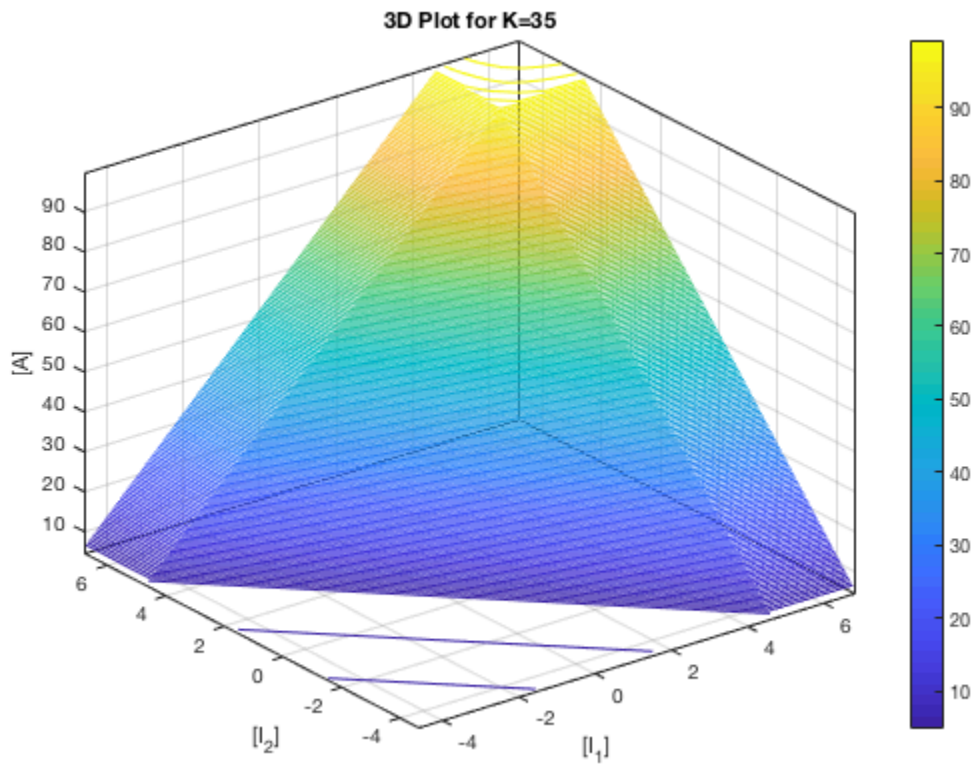
2d)

```
I_1=0.01:100:1000;
I_2=0.01:100:1000;
points=length(I_1);
Aconc=zeros(length(I_1),length(I_2));
for j=1:points
    for i=1:points
        syms A I1 I2
        I1=I_1(j);
        I2=I_2(i);
        eqn=A.*(1+175/((1+I1).*(35+A)-5.*A))+175./
        ((1+I2).*(35+A)-5.*A))==100;
        sol=solve(eqn,A);
        sol=double(sol);
        sol=sol(sol>=0);
        [m,n]=(size(sol));
        if m>1
```

```

        val=min(sol);
    else
        val=sol;
    end
    Aconc(j,i)=val;
end
end
figure (5)
contour3(log(I_1),log(I_2),Aconc,200);
title('3D Plot for K=35');
colorbar
xlabel(' [I_1] ');
ylabel(' [I_2] ');
zlabel(' [A] ');
% k=35 gives a slower respond compare to the ones from k=5; also from
the
% plot, there are some "unstable" values at the bottle, not very
uniform. Thus, this one is "fuzzy"

```



2e)

The choices of parameter is very important and it affects how sensitive the output with regrad to the input.

Published with MATLAB® R2019a

```
function f=NoInhi(B)
% function for 7770 ps4 #2
% B(1)=[A]; B(2)=[B]; B(3)=[C];
f=[(5.*B(1))./(5+B(1))-B(2)./(5+B(2));
(5.*B(1))./(5+B(1))-B(3)./(5+B(3));
100-B(1)-B(2)-B(3)];
end
```

Not enough input arguments.

Error in NoInhi (line 4)
*f=[(5.*B(1))./(5+B(1))-B(2)./(5+B(2));*

Published with MATLAB® R2019a