ChemE 7770 PS.4 4/24/20

1.

$\frac{\gamma_1}{V_2}[R_T] = 5$

$\frac{\gamma_3}{V_4}[X_T] = 10$

a. solve Y^* as a fcn of $[L]$ at s.s

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

① $k_{on}[R][L] - k_{off}[R^*] = 0$

② $\frac{V_1[X]}{K_1+[X]} - \frac{V_2[X^*]}{K_2+[X^*]} = 0$; $V_1 = \gamma_1[R^*]$

③ $\frac{V_3[Y]}{K_3+[Y]} - \frac{V_4[Y^*]}{K_4+[Y^*]} = 0$, $V_3 = \gamma_3[X^*]$

nondimensionalize:

$x^* = \frac{[X^*]}{X_T}$; $K_1 = \frac{K_1}{X_T}$, $K_2 = \frac{K_2}{X_T}$; $K_3 = \frac{K_3}{Y_T}$; $K_4 = \frac{K_4}{Y_T}$; $K_D = \frac{k_{off}}{(k_{on}[L])}$

$\theta_B = \frac{[R^*]}{R_T}$; $\frac{V_1}{V_2} = \left(\frac{\gamma_1\theta_B}{V_2}\right)R_T$; $\frac{V_3}{V_4} = \left(\frac{\gamma_3 X^*}{V_4}\right)X_T$

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 $\theta_B = \frac{1}{1+K_D}$

②

$\frac{\gamma_1[R^*](X_T - [X^*])}{K_1X_T + (X_T - [X^*])} = \frac{V_2[X^*]}{K_2X_T + [X^*]}$

$\left(\frac{\gamma_1\theta_B}{V_2}\right)R_T(X_T - [X^*])(K_2X_T + [X^*]) = [X^*](K_1X_T + X_T - [X^*])$

$\left(\frac{\gamma_1\theta_B}{V_2}\right)R_T(\cancel{X_T} - x^*\cancel{X_T})(K_2\cancel{X_T} + x^*\cancel{X_T}) = x^*\cancel{X_T}(K_1\cancel{X_T} + \cancel{X_T} - x^*\cancel{X_T})$

$\left(\frac{\gamma_1\theta_B}{V_2}\right)R_T(1-x^*)(K_2 + x^*) = x^*(K_1 + 1 - x^*)$

$\underbrace{\left(1-\frac{V_1}{V_2}\right)}_{a}x^{*2} + \underbrace{\left(\frac{V_1}{V_2} - \frac{V_1}{V_2}K_2 - K_1 - 1\right)}_{b}x^* + \underbrace{\frac{V_1}{V_2}K_2}_{c} = 0$

$x^* = \frac{\left(\frac{V_1}{V_2}K_2 + K_1 + 1 - \frac{V_1}{V_2}\right) \pm \sqrt{\left(\frac{V_1}{V_2} - \frac{V_1}{V_2}K_2 - K_1 - 1\right)^2 - 4\left(1-\frac{V_1}{V_2}\right)\left(\frac{V_1}{V_2}K_2\right)}}{2\left(1-\frac{V_1}{V_2}\right)}$

where $\frac{V_1}{V_2} = \frac{\gamma_1\theta_B}{V_2}R_T$

③.

$\frac{\frac{V_3}{V_4}(Y_T - [Y^*])}{K_3Y_T + (Y_T - [Y^*])} - \frac{[Y^*]}{K_4Y_T + [Y^*]} = 0$

$\frac{\frac{V_3}{V_4}(\cancel{Y_T} - y^*\cancel{Y_T})}{K_3\cancel{Y_T} + (\cancel{Y_T} - y^*\cancel{Y_T})} - \frac{y^*\cancel{Y_T}}{K_4\cancel{Y_T} + y^*\cancel{Y_T}} = 0$

$\frac{\frac{V_3}{V_4}(1-y^*)}{K_3 + (1-y^*)} - \frac{y^*}{K_4 + y^*} = 0.$

Simplify:

$\underbrace{\left(1-\frac{V_3}{V_4}\right)}_{a}y^{*2} + \underbrace{\left(\frac{V_3}{V_4} - \frac{V_3}{V_4}K_4 - K_3 - 1\right)}_{b}y^* + \underbrace{\frac{V_3}{V_4}K_4}_{c} = 0$

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

$y^* = \frac{\left(1 + K_3 + \frac{V_3}{V_4}K_4 - \frac{V_3}{V_4}\right) \pm \sqrt{\left(\frac{V_3}{V_4} - \frac{V_3}{V_4}K_4 - K_3 - 1\right)^2 - 4\left(1-\frac{V_3}{V_4}\right)\left(\frac{V_3}{V_4}K_4\right)}}{2\left(1-\frac{V_3}{V_4}\right)}$

where $\frac{V_3}{V_4} = \frac{\gamma_3 X^*}{V_4}X_T$

$K = 10$

1 b) $K_1 = K_2 = K_3 = K_4 = K$, $K = 0.1$ & $K = 10$ plot θ_B, x^* and y^* v.s $\frac{1}{K_D}$. Given. $\frac{\gamma_1}{V_2}[R_T] = 5$

$\frac{\gamma_3}{V_4}[X_T] = 10$

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

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

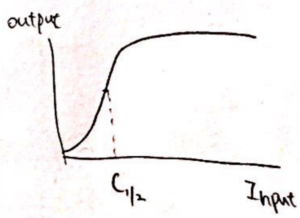
$\frac{V_1}{V_2} = \frac{\gamma_1 \theta_B}{V_2} R_T = 5 \cdot \theta_B$

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

$\frac{V_3}{V_4} = \frac{\gamma_3 x^*}{V_4} X_T = 10x^*$

(plot showed in matlab.)

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



using Excel Regression fitting. get.

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

↑ 3rd parameter (if necessary)

$K = 0.1$

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

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

$1/K_D$ v.s y^* : $n = 7.08$; $C_{1/2} = 0.245$ $\quad m = 0.992$

$K = 10$

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

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

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

d). changes calculated from matlab.

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

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

e). See answer in matlab.

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2.

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

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

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

① $V_1 - V_3 = 0$

② $V_2 - V_4 = 0$ $\Rightarrow$

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

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

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

② $$\frac{V_{max2}[A]}{\left(1 + \cancel{\frac{[I_2]}{K_{I2}}}\right)(K_{S2} + [A])} - \frac{V_{max4}[C]}{\underset{\to K_{S4}?}{K_{S3}} + [C]} = 0$$

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

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

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

Problem 1

1a)

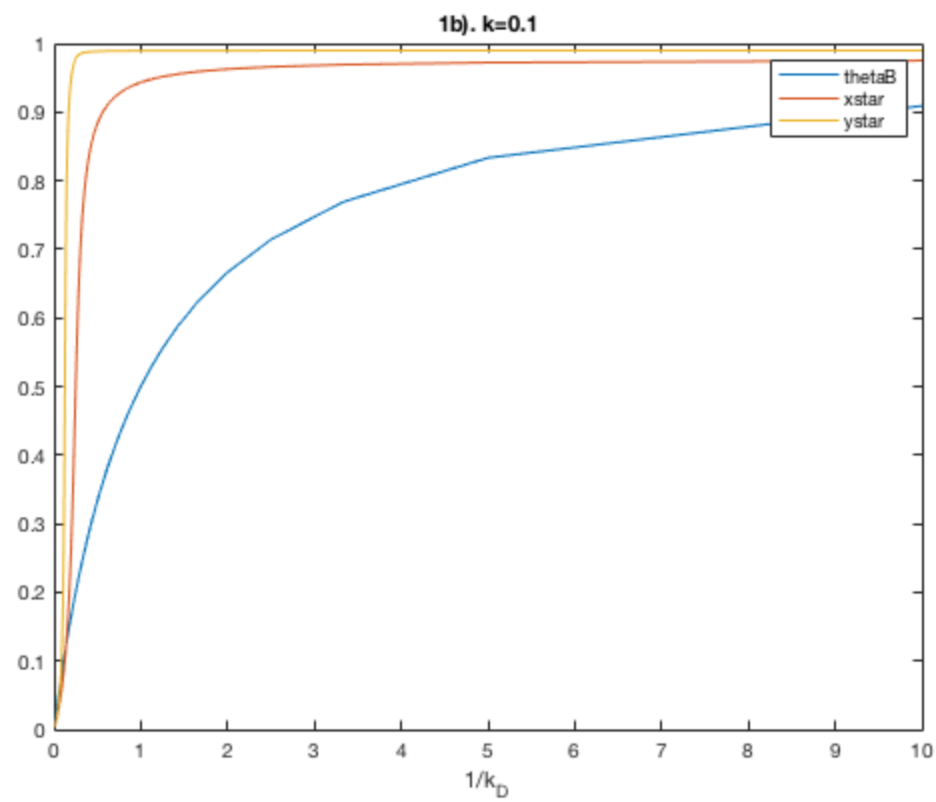
See the attached paper for calculation steps.

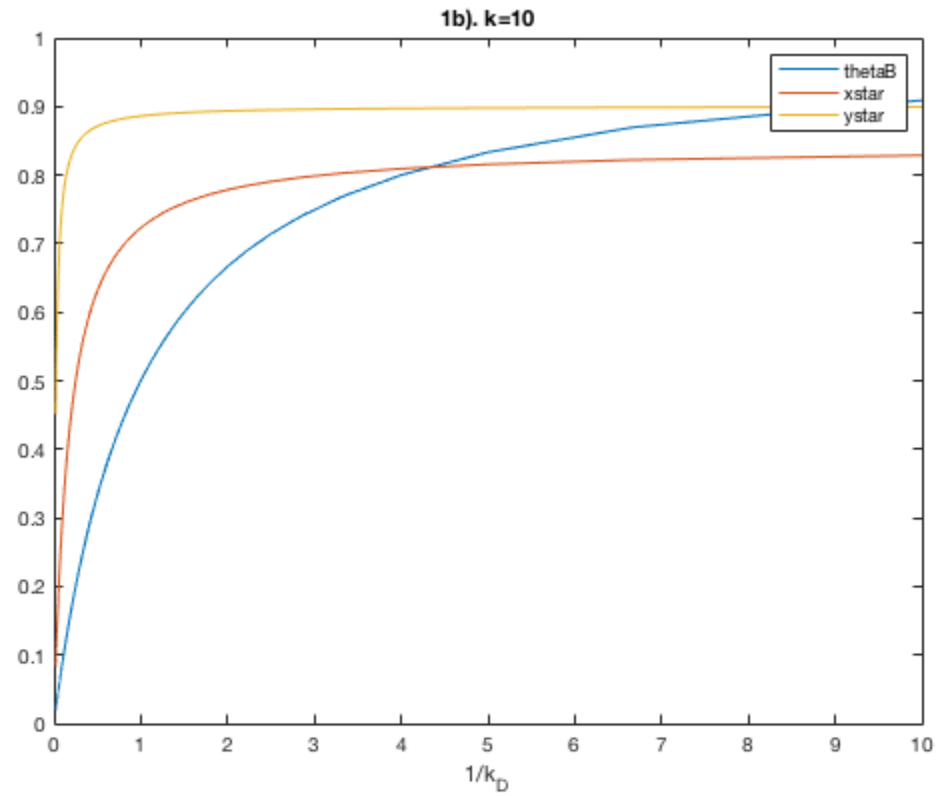
1b).

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/kd vs thetaB, xstar, ystar 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 kd 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
 respectivly: ',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 respectivly:
 ',num2str(thetaB_ch2),'%, ',num2str(xstar_ch2),'%, and
 ',num2str(ystar_ch2),'%']);
```

```
% change of thetaB, xstar, and ystar for k=0.1 respectivly: 43.4783%,
 101.8261%, and 402.5798%
% change of thetaB, xstar, and ystar for k=10 respectivly: 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)

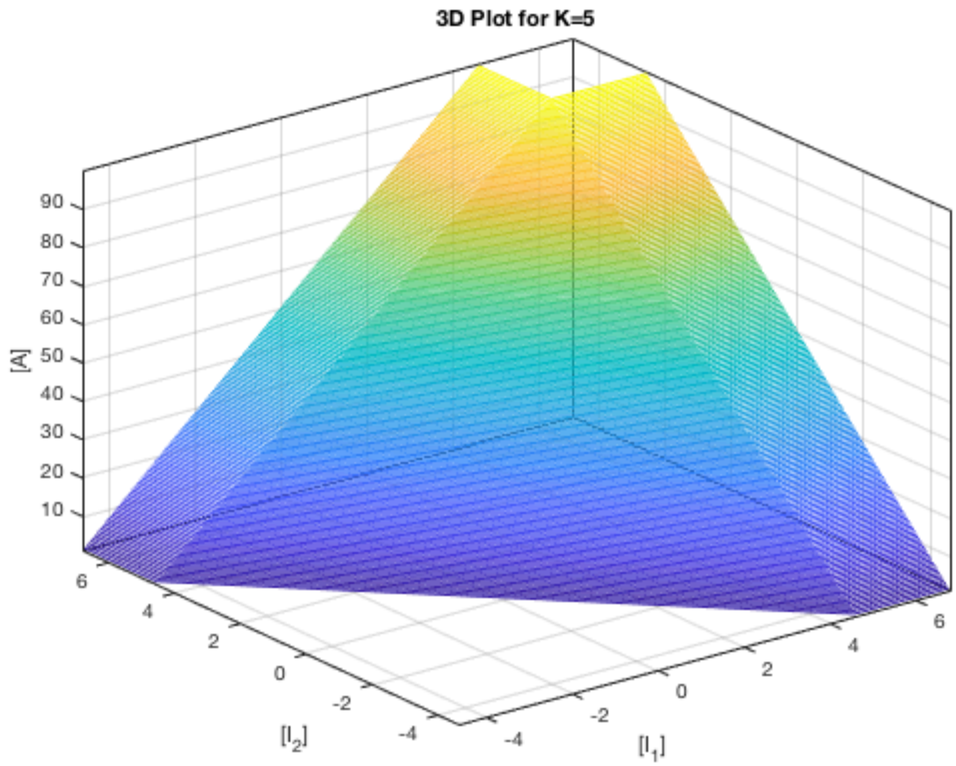
```
B0=[4 4 6]';
[Soln,fval,exit,output]=fsolve(@NoInhi,B0);
display(Soln);
```

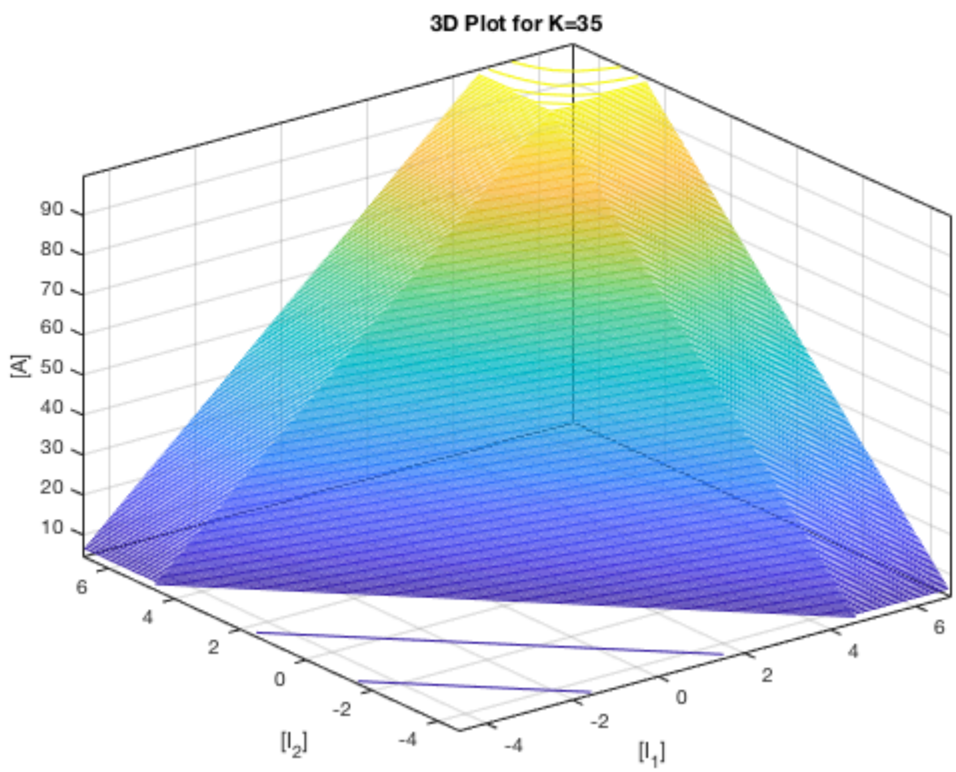
```
Equation solved.

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);
title('3D Plot for K=5');
xlabel('[I_1]');
ylabel('[I_2]');
```

```
zlabel('[A]');
% 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');
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"
```


3D Plot for K=5
[A]
[I_2]
[I_1]


3D Plot for K=35
[A]
[I_2]
[I_1]

2e)

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

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```
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
```