

HW#7

### 1. For 4<sup>th</sup> edition

m-Xylene  $\rightarrow$  Benzene + Methane

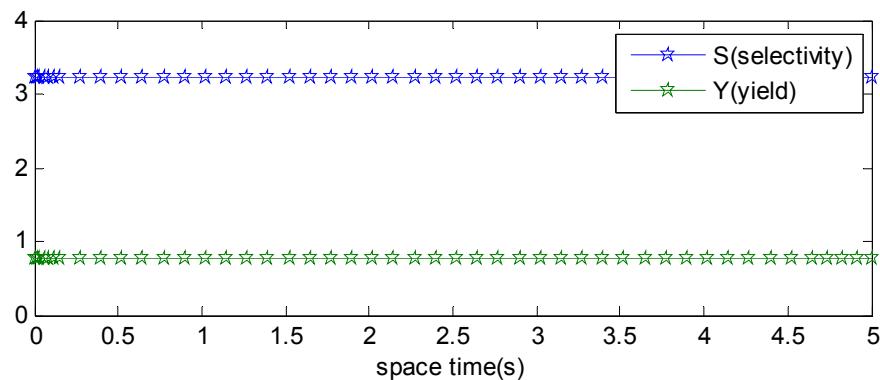
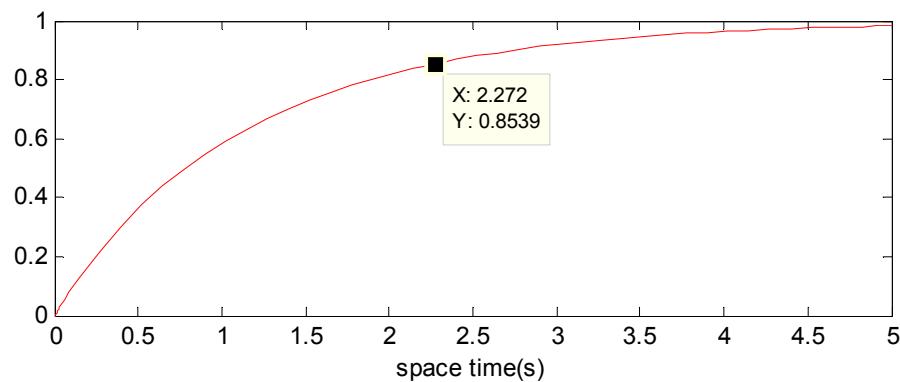


m-Xylene  $\rightarrow$  p-xylene



For 85% conversion  $\tau=2.27$  s

( for 3<sup>rd</sup> edition  $\tau=2.8$ s)



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```
%filename run_P6_12_a.m
clear
global k1 k2 FI CTo vo
k1=0.22; % in 1/s
k2=0.71; % in 1/s
vo=200; % in dm^3/s
CTo=0.05;%in mol/dm^3
```

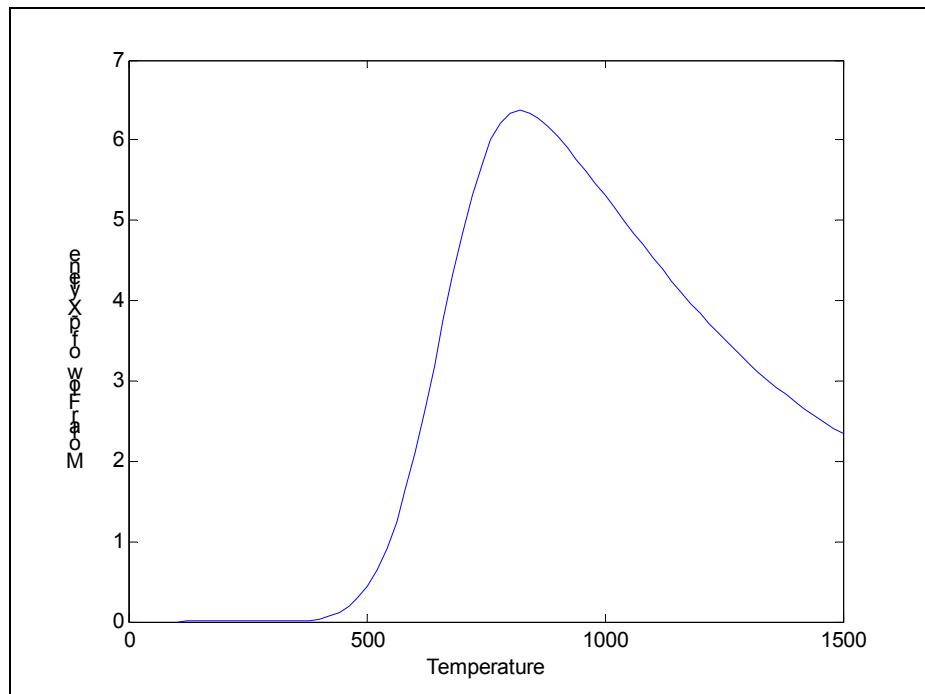
```

C1o=0.75*CTo; % in mol/dm^3
FI=0.25*CTo*vo; % in mol/s
F1o=C1o*vo; % in mol/s
Fo(1)=F1o;
Fo(2)=0;
Fo(3)=0;
Fo(4)=0;
tspan=[0 5];
[t,F]=ode45('ode_P6_12_a',tspan,Fo);
F1=F(:,1);
F2=F(:,2);
F3=F(:,3);
F4=F(:,4);
%X=(F1o-F1)/F1o;
%rr=[t,X];
%plot(t,X,'r')
%xlabel('space time(s)')
%ylabel('X')
S=F4/(F2+0.0000000001)
Y=F4/(F1o+0.0000000001-F1)
plot(t,S,'p-',t,Y,'p-')
legend('S(selectivity)', 'Y(yield)')
xlabel('space time(s)')
=====
% filename ode_P6_12_a.m
function dF_dt=ode_P6_12_a(t,F)
global k1 k2 FI CTo vo
FT=F(1)+F(2)+F(3)+F(4)+FI;
r1=k1*CTo*F(1)/FT;
r2=k2*CTo*F(1)/FT;
dF_dt(1)=(-r1-r2)*vo;
dF_dt(2)=r1*vo;
dF_dt(3)=r1*vo;
dF_dt(4)=r2*vo;
dF_dt=dF_dt';
=====
```

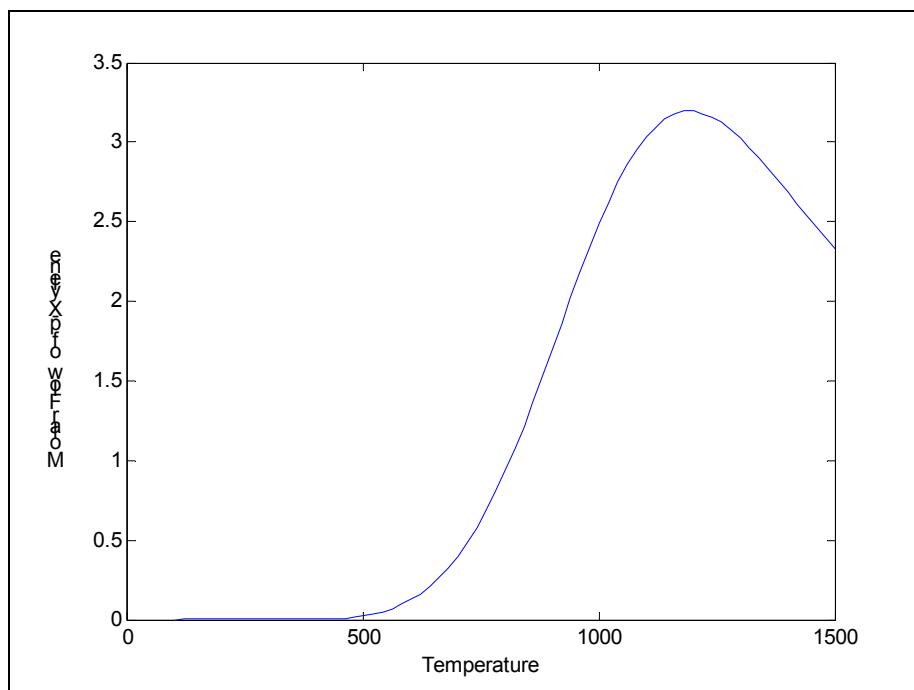
(b) For space time is  $2000/200=10\text{s}$

The ideal temperature is **822K**

**4<sup>th</sup> Edition**



(For 3<sup>rd</sup> edition  $\tau=0.5 \text{ s} \rightarrow$  ideal  $T=1194\text{K}$ )



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```
% filename run_P6_12_b.m
```

```
global k1 k2 C10 tau
```

```
k10=0.22;
```

```

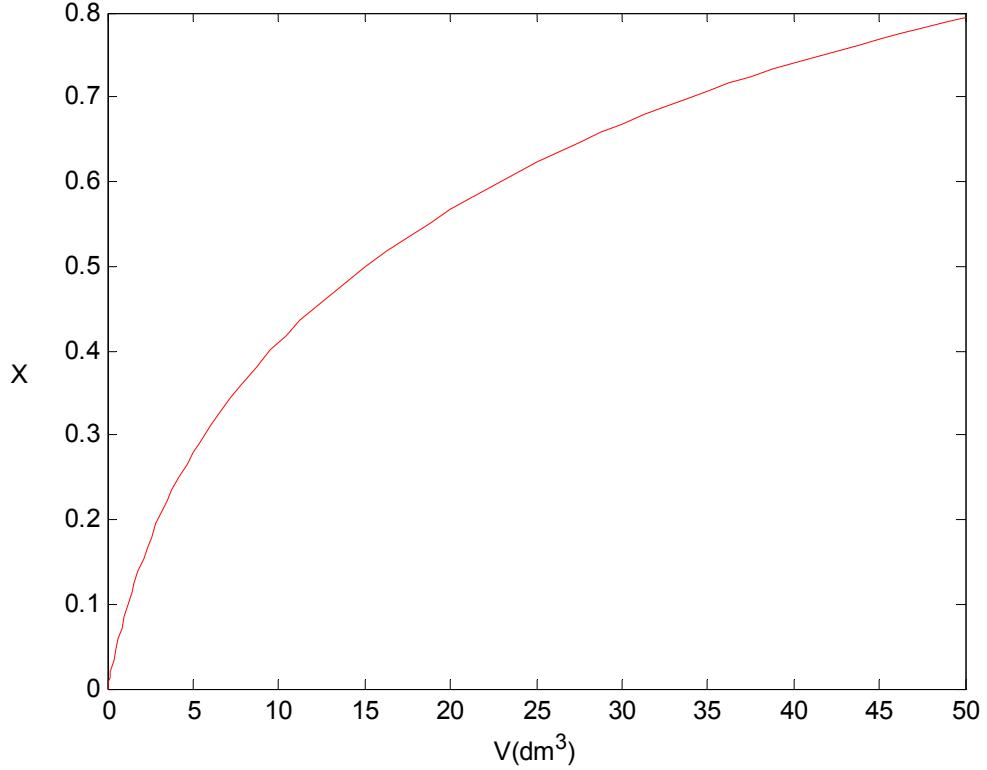
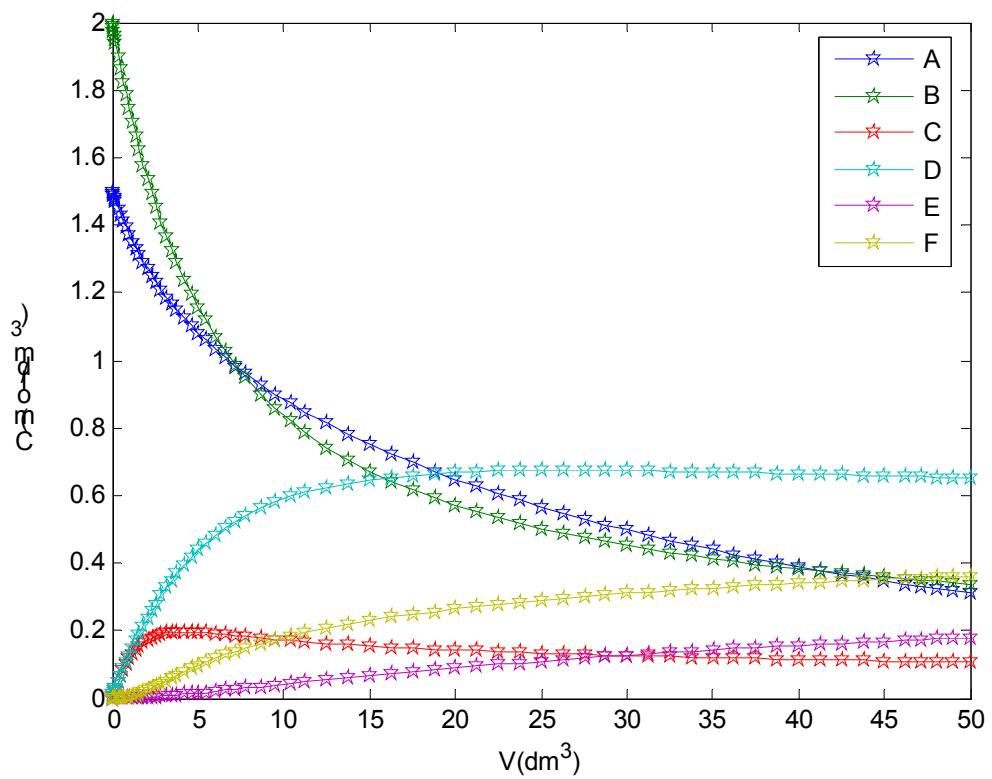
k2o=0.71;
T=880;
k1=k1o*exp(20000/1.987*(1/946-1/T));
k2=k2o*exp(10000/1.987*(1/946-1/T));
tau=10;
C1o=0.0375;
guess=[C1o 0 0 0];
[C]=fsolve('P6_12_b',guess)
CD=C(:,4);
[m,n]=size(CD);
Final=C(m,4)

=====
% P_6_12_b.m
function F=P6_12_b(C)
global k1 k2 C1o tau
%
% For CSTR design equation: Fj0-Fj=-rjV=Cjo*v0-Cj*v0
% First, set up the rate expressions in terms of concentration
%
r1=k1*C(1)
r2=k2*C(1)
%
% Then write mole balances for all species
% using the appropriate stoichiometry
%
F(1)=C(1)-C1o+(r1+r2)*tau % this is mole balance for CA
F(2)=C(2)-r1*tau % this is mole balance for CB
F(3)=C(3)-r1*tau % this is mole balance for CC
F(4)=C(4)-r2*tau % this is mole balance for CD

```

2.

(a)




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```
%filename P6_14_a.m
```

```

global vo k1 k2 k3

k1=0.25; % in dm^6/(mol^2-min)
k2=0.1; % in dm^3/(mol-min)
k3=5.0; % in dm^6/(mol^2-min)
vo=10; % in dm^3/min
C1o=1.5; % in mol/dm^3
C2o=2.0; % in mol/dm^3
Co(1)=C1o;
Co(2)=C2o;
Co(3)=0;
Co(4)=0;
Co(5)=0;
Co(6)=0;
Vspan=[0 50];
[V,C]=ode45('odeP6_14_a',Vspan,Co);
C1=C(:,1);
C2=C(:,2);
C3=C(:,3);
C4=C(:,4);
C5=C(:,5);
C6=C(:,6);

%plot(V,C1,'p-',V,C2,'p-',V,C3,'p-',V,C4,'p-',V,C5,'p-',V,C6,'p-')
%legend('A','B','C','D','E','F')
%xlabel('V(dm^3)')
%ylabel('C(mol/dm^3)')

X=(C1o-C1)/C1o;
plot(V,X,'r')
xlabel('V(dm^3)')
ylabel('X')
=====

%filename odeP6_14_a.m
function dC_dV=odeP6_14_a(V,C)
global vo k1 k2 k3
r1=k1*C(1)*C(2)^2;
r2=k2*C(1)*C(4);
r3=k3*C(2)*C(3)^2;
dC_dV(1)=(-r1-3*r2)/vo;
dC_dV(2)=(-2*r1-r3)/vo;

```

```

dC_dV(3)=(r1+r2-2*r3)/vo;
dC_dV(4)=(r1-2*r2+r3)/vo;
dC_dV(5)=(r2)/vo;
dC_dV(6)=(r3)/vo;
dC_dV=dC_dV'

```

$$(b) \quad C_A = 0.6083 \text{ mol/dm}^3$$

$$C_B = 0.7927 \text{ mol/dm}^3$$

$$C_D = 0.4535 \text{ mol/dm}^3$$

$$C_F = 0.2516 \text{ mol/dm}^3$$

$$X = (1.5 - 0.61) / (1.5) = 0.59$$


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```

% run_P_6_14_b.m
global k1 k2 k3 V C10 C20 v0
%
% rate constant
%
k1=0.25 % in dm^6/mol^2.min
k2=0.1 % in dm^3/mol.min
k3=5.0 % in dm^6/mol^2.min
%
% initial concentration for A and B
%
C10=1.5 % in mol/dm^3
C20=2.0 % in mol/dm^3
%
% reactor volume and initial flow rate
%
V=50 % in dm^3
v0=10 % dm^3/min
%
% guess the answer
%
guess=[1.5 0 0 0 0 0]
%
% call solver
%
[C]=fsolve('P_6_14_b',guess)

```

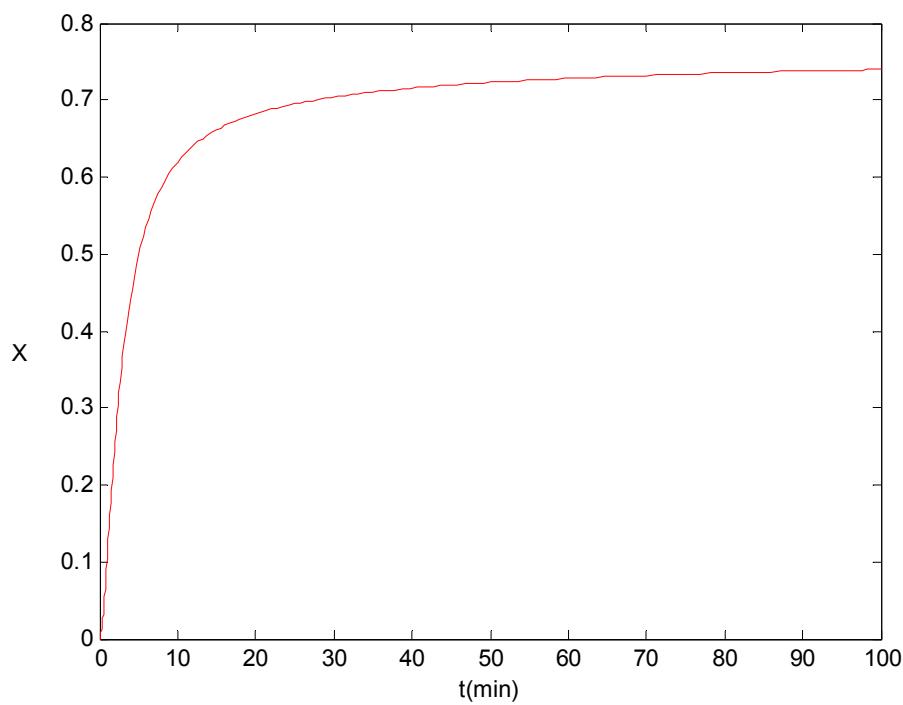
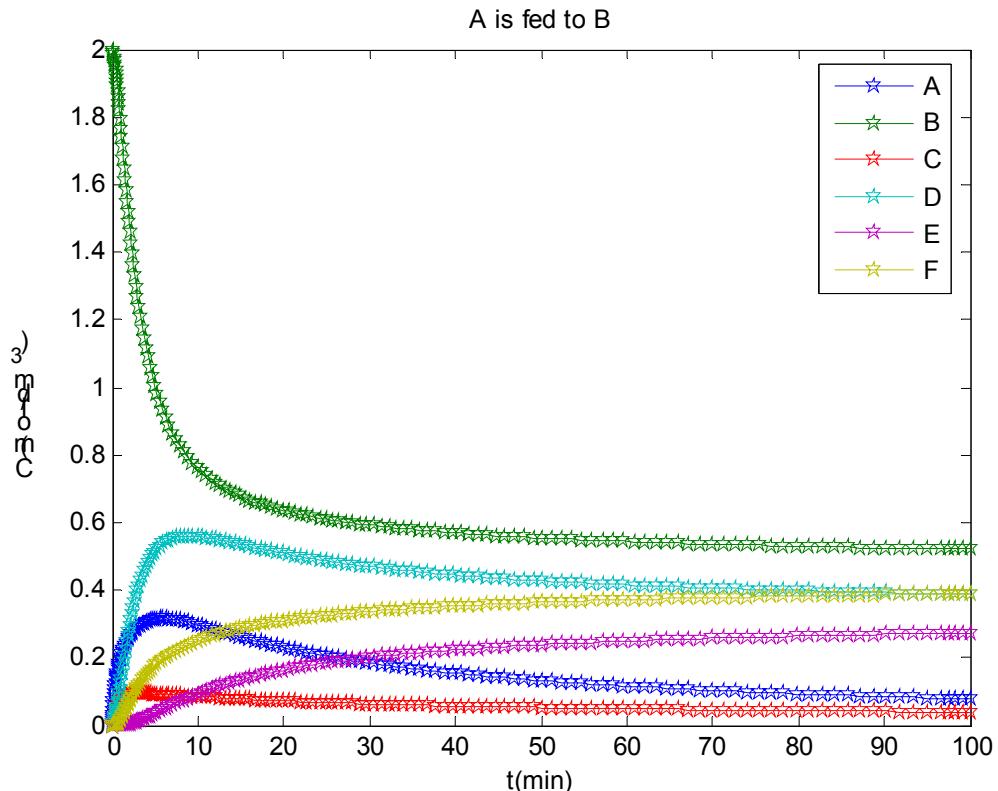
```
=====
% P_6_14_b.m
function F=P_6_14_b(C)
global k1 k2 k3 V C10 C20 v0
%
% For CSTR design equation: Fj0-Fj=-rjV=Cjo*v0-Cj*v0
% First, set up the rate expressions in terms of concentration
%
r1=k1*C(1)*C(2)^2
r2=k2*C(1)*C(4)
r3=k3*C(2)*C(3)^2
%
% Then write mole balances for all species
% using the appropriate stoichiometry
%
F(1)=(C10-C(1))*v0-(r1+3*r2)*V % this is mole balance for CA
F(2)=(C20-C(2))*v0-(2*r1+r3)*V % this is mole balance for CB
F(3)=C(3)*v0-(r1+r2-2*r3)*V % this is mole balance for CC
F(4)=C(4)*v0-(r1-2*r2+r3)*V % this is mole balance for CD
F(5)=C(5)*v0-r2*V % this is mole balance for CE
F(6)=C(6)*v0-r3*V % this is mole balance for CF
```

(c)

(1) A is fed to B

$$C_{A0} = 0$$

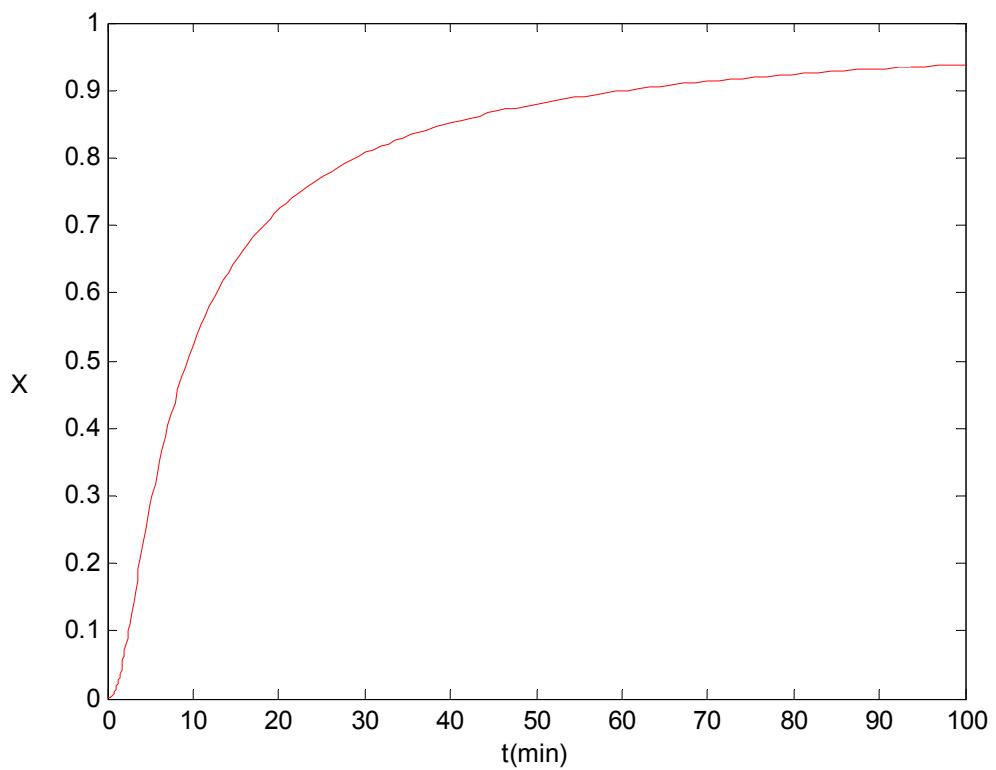
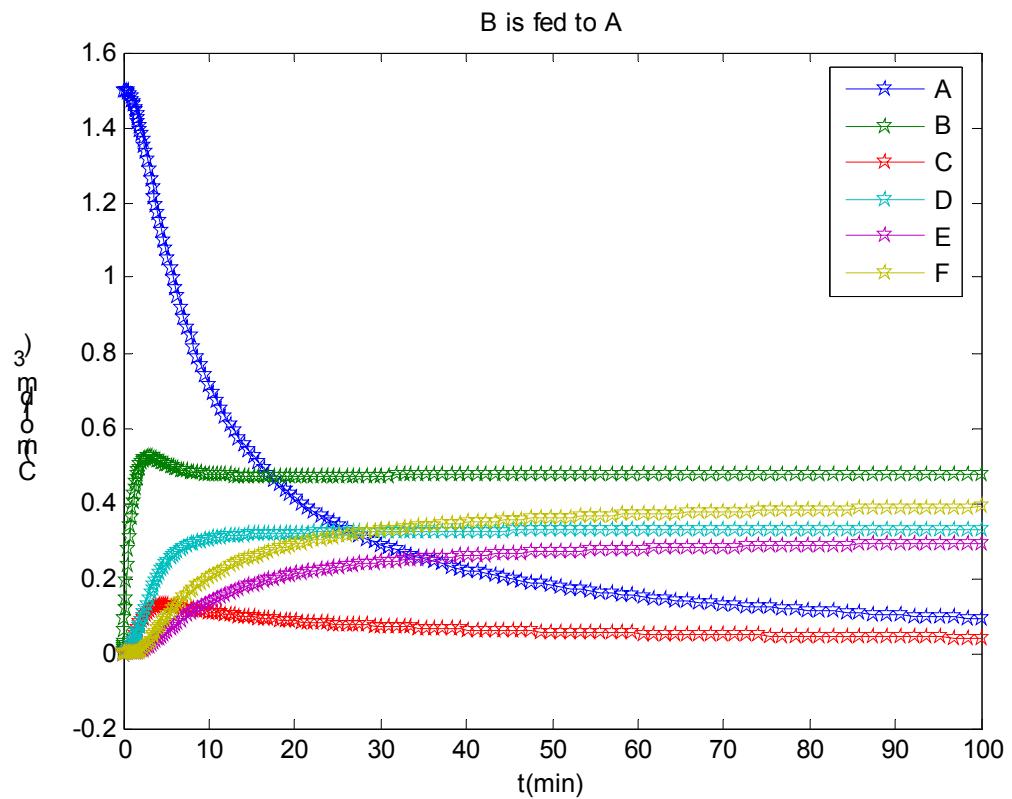
$$C_{B0} = 2.0$$



(2) B is fed to A

$$C_{A0} = 1.5$$

$$C_{B0} = 0$$




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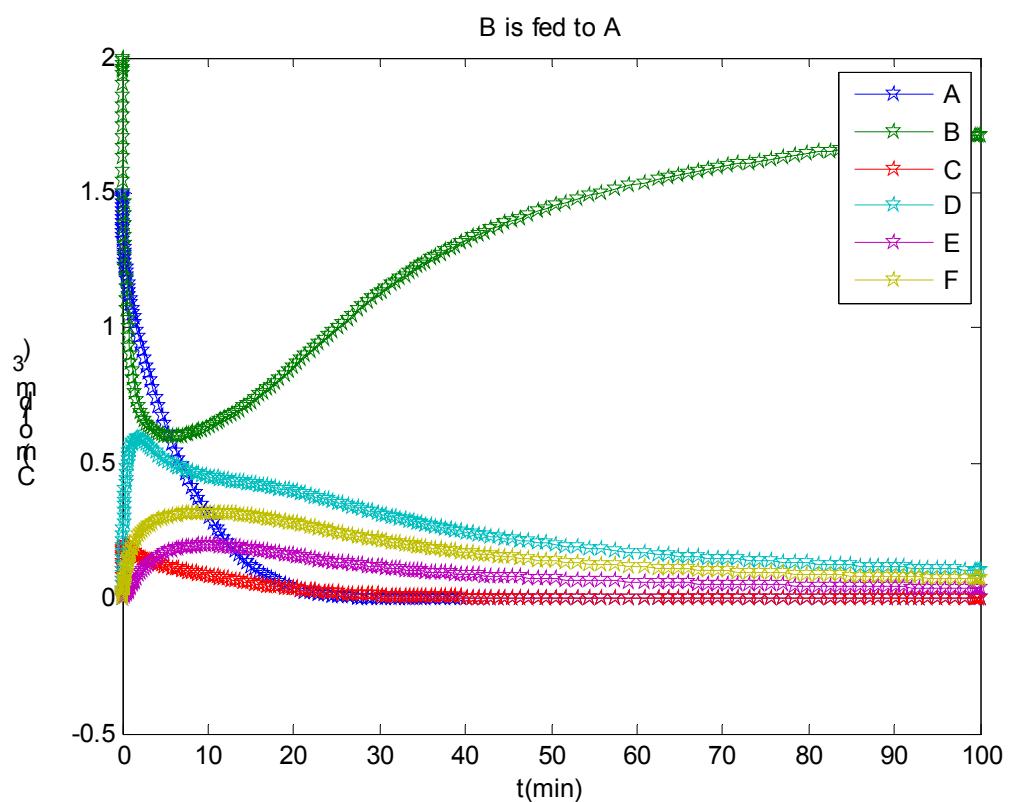
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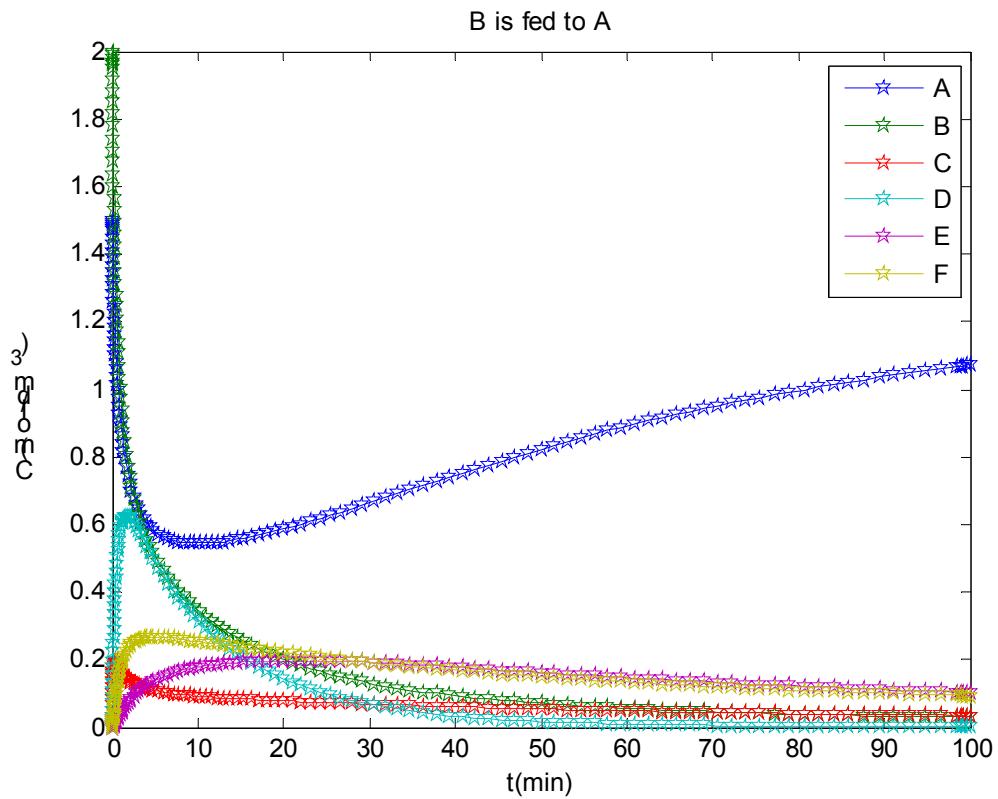
```

%filename P6_14_c.m
global vo k1 k2 k3 Vo C1o C2o
k1=0.25; % in dm^6/(mol^2-min)
k2=0.1; % in dm^3/(mol-min)
k3=5.0; % in dm^6/(mol^2-min)
vo=10; % in dm^3/min
Vo=40; % in dm^3
C1o=1.5; % in mol/dm^3
C2o=2.0; % in mol/dm^3
Co(1)=C1o;
Co(2)=0;
Co(3)=0;
Co(4)=0;
Co(5)=0;
Co(6)=0;
Co(7)=Vo;
tspan=[0 100];
[t,C]=ode45('odeP6_14_c',tspan,Co);
C1=C(:,1);
C2=C(:,2);
C3=C(:,3);
C4=C(:,4);
C5=C(:,5);
C6=C(:,6);
C7=C(:,7);
plot(t,C1,'p-',t,C2,'p-',t,C3,'p-',t,C4,'p-',t,C5,'p-',t,C6,'p-')
legend('A','B','C','D','E','F')
xlabel('t(min)')
ylabel('C(mol/dm^3)')
title('B is fed to A')
%X=(C1o-C1)/C1o;
%plot(t,X,'r')
%xlabel('t(min)')
%ylabel('X')
=====
```

```
%filename odeP6_14_c.m
function dC_dt=odeP6_14_c(t,C)
global vo k1 k2 k3 Vo C1o C2o
r1=k1*C(1)*C(2)^2;
r2=k2*C(1)*C(4);
r3=k3*C(2)*C(3)^2;
dC_dt(1)=(-r1-3*r2)+(C1o-C(1))/C(7)*vo;
dC_dt(2)=(-2*r1-r3)+(C2o-C(2))/C(7)*vo;
dC_dt(3)=(r1+r2-2*r3)-C(3)/C(7)*vo;
dC_dt(4)=(r1-2*r2+r3)-C(4)/C(7)*vo;
dC_dt(5)=r2-C(5)/C(7)*vo;
dC_dt(6)=r3-C(6)/C(7)*vo;
dC_dt(7)=vo;
dC_dt=dC_dt '
```

3<sup>rd</sup> Edition A->B





(d) As  $\theta_B$  increases the outlet concentrations of species D and F increase, while the outlet concentrations of species A, C and E decrease. When  $\theta_B$  is large, reaction 1 and 3 are favored and when it is small the rate of reaction 2 will increase.