ENVE404: Environmental Modeling

Homework 5

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Question 1)

a)

Mass Balances

$$\frac{dC_{A1}}{dt} = C_{A0}/t_d - C_{A1}/t_d - k_1 C_{A1} + k_{-1} C_{B1}$$

$$\frac{dC_{B1}}{dt} = -C_{B1}/t_d + k_1 C_{A1} - k_{-1} C_{B1}$$

$$\frac{dC_{A2}}{dt} = C_{A1}/t_d - C_{A2}/t_d - k_1 C_{A2} + k_{-1} C_{B2}$$

$$\frac{dC_{B2}}{dt} = C_{B1}/t_d - C_{B2}/t_d + k_1 C_{A2} - k_{-1} C_{B2}$$

b)

Script

```
clc
clear all
close all

tspan = [0:10]; %time span
ci = [0 0 0 0]; %intial concentrations
[t,c] = ode45(@reactions,tspan,ci); %using ode45 to solve

%plotting time vs concentration
plot(t,c)
xlabel('Time (min)')
ylabel('Concentration (mg/L)')
legend('A1','B1','A2','B2','location','southeast')

%creating table for concentrations in first 10 mins
varN = {'Time (min)','A1 (mg/L)','B1 (mg/L)','A2 (mg/L)','B2 (mg/L)'};
T = table(t,c(:,1),c(:,2),c(:,3),c(:,4),'VariableNames',varN);
disp(T)

fprintf('Concentration of A in Reactor 1: %8.4f mg/L\n', c(end,1))
fprintf('Concentration of B in Reactor 1: %8.4f mg/L\n', c(end,2))
fprintf('Concentration of A in Reactor 2: %8.4f mg/L\n', c(end,3))
fprintf('Concentration of B in Reactor 2: %8.4f mg/L\n', c(end,4))
```

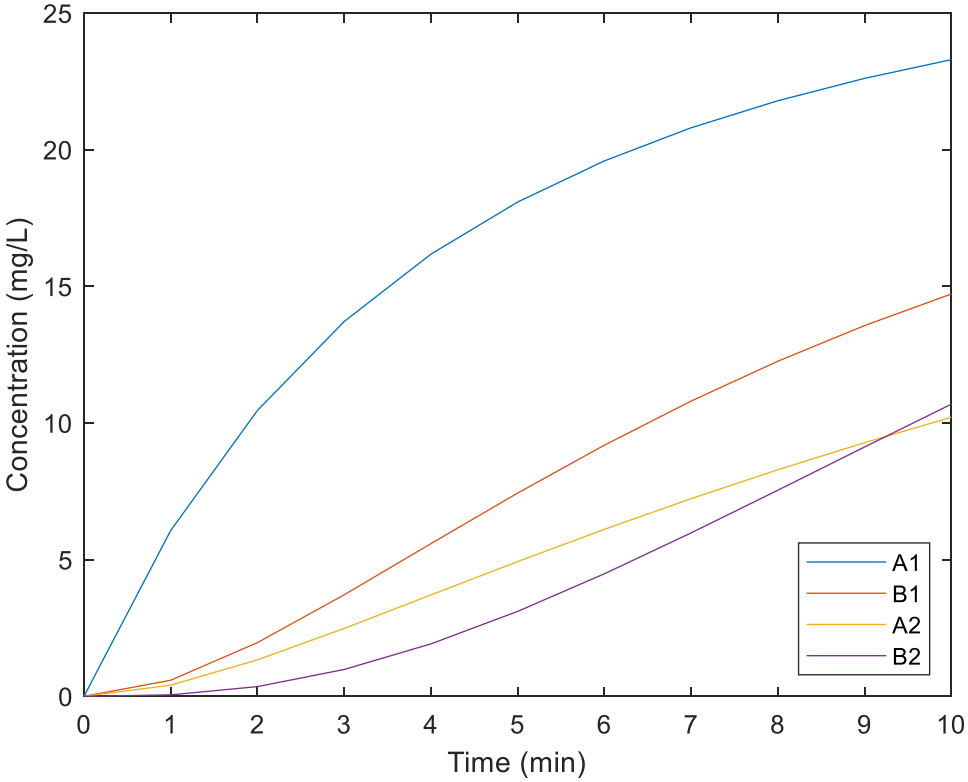
Function

```
function csol = reactions(t,c)

td = 7; %residence time
A0 = 50;    %inlet A concentration
k1 = 0.2;   %forward reaction rate coefficient
k2 = 0.1;   %backward reaction rate coefficient

%equations for reactor 1
csol(1) = A0/td-c(1)/td-k1*c(1)+k2*c(2);    %A1
csol(2) = -c(2)/td+k1*c(1)-k2*c(2); %B1
%equations for reactor 2
csol(3) = c(1)/td-c(3)/td-k1*c(3)+k2*c(4);  %A2
csol(4) = c(2)/td-c(4)/td+k1*c(3)-k2*c(4);  %B2

csol =csol(:);
end
```

Results

Time (min)	A1 (mg/L)	B1 (mg/L)	A2 (mg/L)	B2 (mg/L)
0	0	0	0	0
1	6.066	0.59008	0.40929	0.054827
2	10.46	1.966	1.3346	0.35611
3	13.714	3.7139	2.4856	0.98301
4	16.178	5.5856	3.71	1.9193
5	18.086	7.4371	4.9306	3.1087
6	19.592	9.1892	6.1101	4.4839
7	20.804	10.802	7.232	5.9801
8	21.793	12.262	8.2899	7.5415
9	22.612	13.565	9.2824	9.1229
10	23.297	14.721	10.21	10.689

```
Concentration of A in Reactor 1:  23.2969 mg/L
Concentration of B in Reactor 1:  14.7206 mg/L
Concentration of A in Reactor 2:  10.2105 mg/L
Concentration of B in Reactor 2:  10.6891 mg/L
```


25
20
15
10
5
0
Concentration (mg/L)
0
1
2
3
4
5
6
7
8
9
10
Time (min)
A1
B1
A2
B2

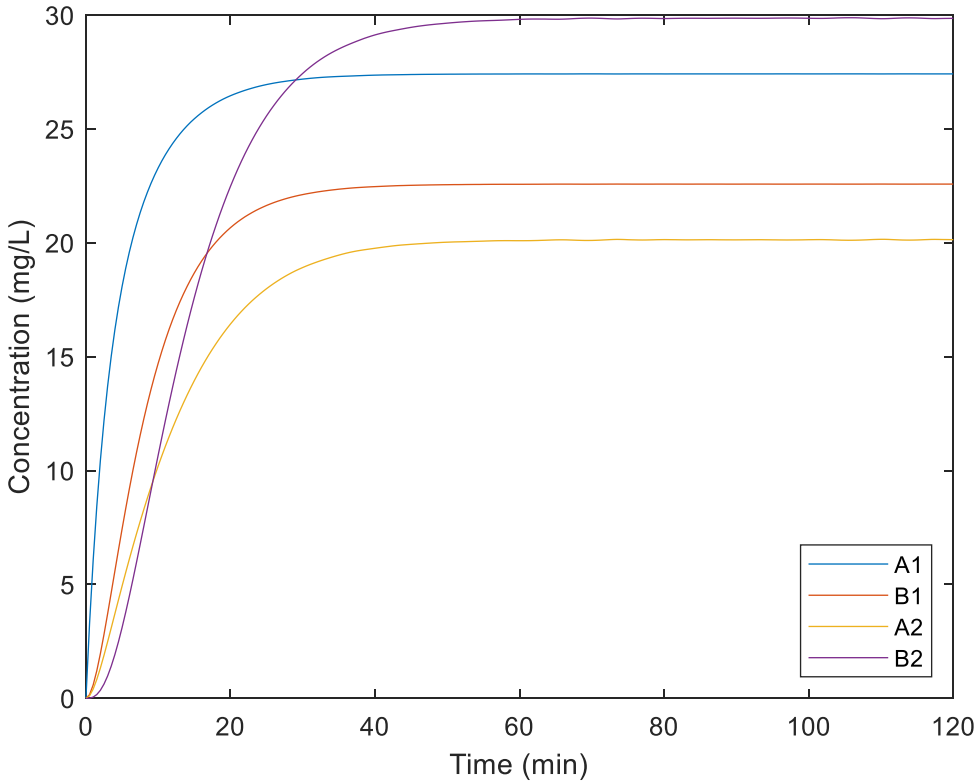
c)

Script

```
clc
clear all
close all

tspan = [0:0.5:120]; %time span
ci = [0 0 0 0]; %intial concentrations
[t,c] = ode45(@reactions,tspan,ci); %using ode45 to solve

%finding time to reach steady state
c = round(c,3);
for i = 1:length(t)
    if c(i,1)==c(end,1)&&c(i,2)==c(end,2)&&c(i,3)==c(end,3)&&c(i,4)==c(end,4)
        ss = i;
        break
    end
end

plot(t,c)
xlabel('Time (min)')
ylabel('Concentration (mg/L)')
legend('A1','B1','A2','B2','location','southeast')

fprintf('Time until steady state: %8.3f min\n', t(ss))
fprintf('Steady state concentration of A in Reactor 1: %8.3f mg/L\n', c(ss,1))
fprintf('Steady state concentration of B in Reactor 1: %8.3f mg/L\n', c(ss,2))
fprintf('Steady state concentration of A in Reactor 2: %8.3f mg/L\n', c(ss,3))
fprintf('Steady state concentration of B in Reactor 2: %8.3f mg/L\n', c(ss,4))
```

Results

```
Time until steady state:  108.500 min
Steady state concentration of A in Reactor 1:   27.419 mg/L
Steady state concentration of B in Reactor 1:   22.581 mg/L
Steady state concentration of A in Reactor 2:   20.141 mg/L
Steady state concentration of B in Reactor 2:   29.859 mg/L
```



Question 2)

a)

Steady-state Mass Balances

$$0 = \frac{dC_{NH_3}}{dt} = -\frac{Q}{A}\frac{dC_{NH_3}}{dx} - k_1 C_{NH_3}$$

$$0 = \frac{dC_{NO_2}}{dt} = -\frac{Q}{A}\frac{dC_{NO_2}}{dx} + k_1 C_{NH_3} - k_2 C_{NO_2}$$

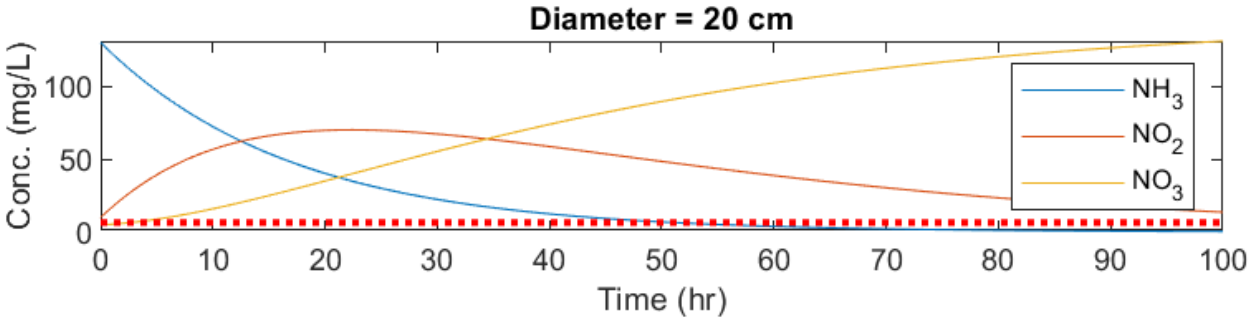
$$0 = \frac{dC_{NO_3}}{dt} = -\frac{Q}{A}\frac{dC_{NO_3}}{dx} + k_2 C_{NO_2}$$

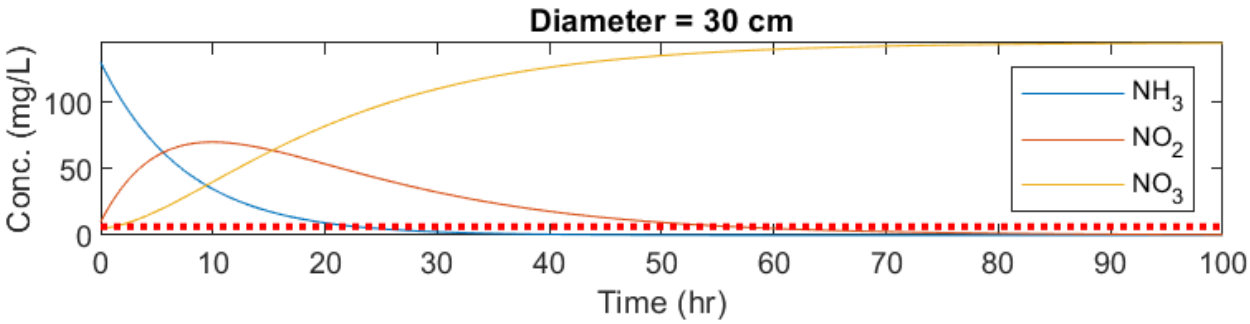
b)

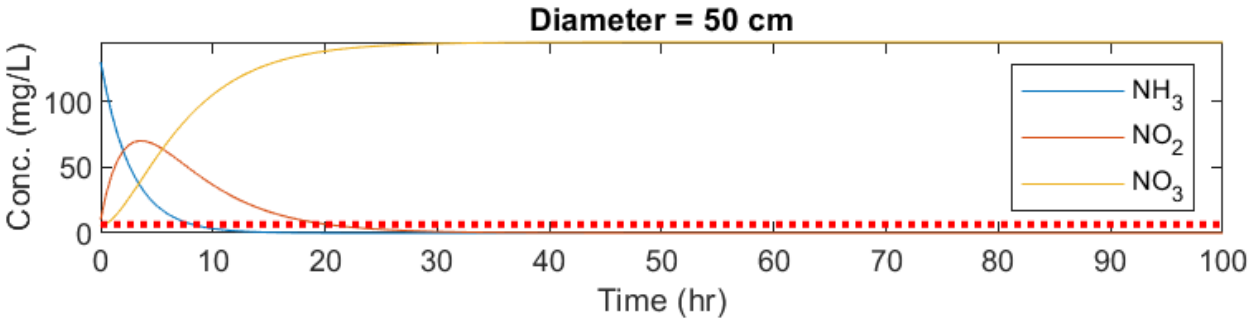
Script

```
clc
clear all
close all

k1 = 0.56;  %NH3 to NO2
k2 = 0.28;  %NO2 to NO3

cin = [130 10 5];   %in mg/L

Q = 300;    %flowrate in L/hr
Q = Q*0.001;    %in m^3/hr

dia = [20 30 50]; %diameters in cm
dia = dia*0.01; %in m

xspan = [0:0.5:100];    %length values in m

for i = 1:length(dia)

    A = pi*(dia(i)/2)^2;    %cross sectional area in m^2

    %function to solve mass balances
    f = @(x,c) [k1*c(1)*(-A/Q);(k2*c(2)-k1*c(1))*(-A/Q);-k2*c(2)*(-A/Q)];
    [x,c] = ode45(f,xspan,cin);

    %plotting time vs concentrations
    subplot(3,1,i)
    plot(x,c)
    hold on
    plot(x,ones(length(x))*(c(1)*0.05),'r:','LineWidth',2)
    title(sprintf('Diameter = %d cm',dia(i)*100))
    xlabel('Time (hr)')
    ylabel('Conc. (mg/L)')
    legend('NH_3','NO_2','NO_3','location','east')
end
```

Results


Diameter = 20 cm
Conc. (mg/L)
0
50
100
0
10
20
30
40
50
60
70
80
90
100
Time (hr)
NH3
NO2
NO3


Diameter = 30 cm
Conc. (mg/L)
0
50
100
0
10
20
30
40
50
60
70
80
90
100
Time (hr)
NH3
NO2
NO3


Diameter = 50 cm
Conc. (mg/L)
0
50
100
0
10
20
30
40
50
60
70
80
90
100
Time (hr)
NH3
NO2
NO3

c)

Script

```
clc
clear all
close all

k1 = 0.56;  %NH3 to NO2
k2 = 0.28;  %NO2 to NO3

cin = [130 10 5];   %in mg/L

Q = 300;    %flowrate in L/hr
Q = Q*0.001;    %in m^3/hr

dia = [20 30 50]; %diameters in cm
dia = dia*0.01; %in m

xspan = [0:0.5:100];    %length values in m

fprintf('The required volumes for 95%% NH3 removal:\n')
for i = 1:length(dia)

    A = pi*(dia(i)/2)^2;    %cross sectional area in m^2

    %function to solve mass balances
    f = @(x,c) [k1*c(1)*(-A/Q);(k2*c(2)-k1*c(1))*(-A/Q);-k2*c(2)*(-A/Q)];
    [x,c] = ode45(f,xspan,cin);

    %finding required volumes
    for j = 1:length(x)
        if cin(1)*0.05 > c(j,1)
            v(i) = A*x(j);
            break
        end
    end

    fprintf('For %d cm diameter: %8.4f m^3\n',dia(i)*100,v(i))
end

%selecting design scenario
for k = 1:length(v)
    if v(k)==min(v)
        fprintf('The design diameter: %d cm\n',dia(k)*100)
        fprintf('The design volume: %8.4f m^3\n',v(k))
    end
end
```

Results

```
The required volumes for 95% NH3 removal:
For 20 cm diameter:   1.6179 m^3
For 30 cm diameter:   1.6258 m^3
For 50 cm diameter:   1.6690 m^3
The design diameter: 20 cm
The design volume:   1.6179 m^3
```