Lab Report 4

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1st Problem

Assignment

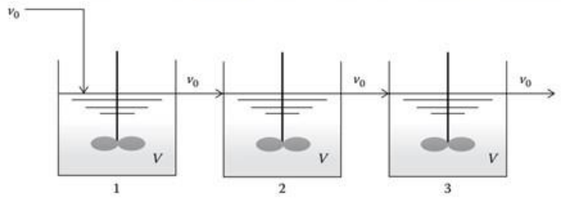
A gas-phase catalytic reaction

$$A \rightarrow B$$

is carried out in a packed bed reactor where the catalyst activity is decaying. The reaction with deactivation follows the rate expression given by

$$-r_A = kaC_A$$

where a is the catalyst activity. The packed bed reactor can be approximated by three CSTRs in series as shown in



Changes in the concentration of A and B in each of the three reactors can be represented as

$$\frac{dC_{Ai}}{dt} = \frac{v_0}{V}\left(C_{A(i-1)} - C_{A(i)}\right) + r_{Ai}, \quad \frac{dC_{Bi}}{dt} = \frac{v_0}{V}\left(C_{B(i-1)} - C_{B(i)}\right) - r_{Ai}$$

A. It is assumed that the catalyst activity follows the deactivation kinetics given by
Plot the concentration of A in each of the three reactors as a function of time to 60 minutes ($0 \le t \le 60$).

$$\frac{da_i}{dt} = -k_d a_i \quad (i = 1,2,3)$$

B. It is assumed that the catalyst activity function is given by
Plot the concentration of *A* in each of the three reactors as a function of time to 60 min ($0 \le t \le 60$).

$$\frac{da_i}{dt} = -k_d a_i C_{B(i)} \quad (i = 1,2,3)$$

Problem 2:

Consider a CSTR of volume 100m^3 with elementary reaction:

A -> B ΔH = -5 × 10^4 J (exothermic reaction)

The rate constant of the reaction is 7.2 × 10^{10} /sec. A cooling jacket is maintained around CSTR to reduce the heat formed due to the reaction. Species A is fed into the reactor at 350 K with a flow rate of 100m^3/s of concentration of 1 mol/m^3. The mixture's overall density is 1000kg/m^{3,} and the heat capacity is 0.239 J/Kg/K.

The activation energy of the reaction is 8750R J/mol. Initial steady-state conditions are 324.48 K, and the concentration is 0.877 mol/m^3. The cooling jacket temperature was initially set as 300 K. Plot the concentration and temperature plots with respect to time up to 5 sec.

Data:

k_d = 0.01 min-1, k = 0.9 dm^3/(dm^3(cat)·min), C_{A0} = 0.01 gmol/cm^3, C_{B0} = 0, v_0= 5 dm^3/ min, V = 10 dm^3, a_i(0) = = 1.0 (i=1,2,3), C_{Ai} (0)= C_{Bi} (0)= 0 (i=1,2,3)

Solution 1 (A): -

Algorithm:-

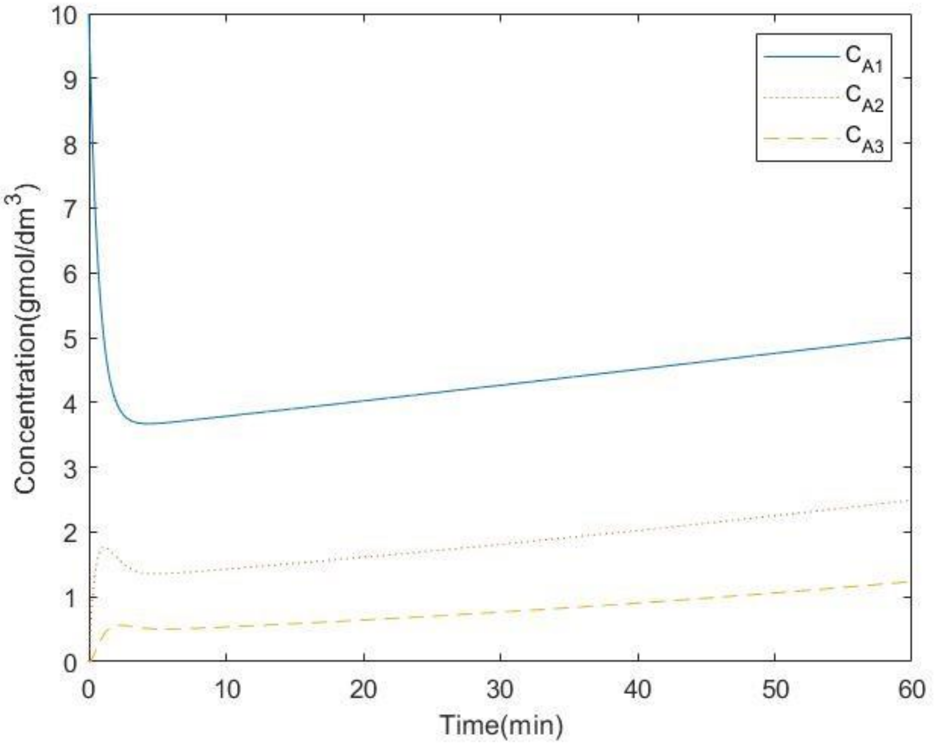
- First we initialise all the parameters.
- Then since the activity coefficient is independent of concentrations of A and B we create an array y of size 6, where y(1), y(2) and y(3) store C_{A1}, C_{A2} and C_{A3} respectively and y(4), y(5) and y(6) store a_1 , a_2 and a_3 respectively.
- Next we define the function dydt which returns a 1d array of size 6 whose ith index stores the differential equation for ith variable y(i).
- Then we use the built-in ode45 method for solving the system of ODEs.
- Finally we plot graphs of 1st, 2nd and 3rd columns of y vs time where 1st column stores values of C_{A1}, 2nd column stores values of C_{A2} and third column stores values of C_{A3} respectively.

Code: -

```
%initial conditions
v0 = 5; %inlet flow rate
V = 10; %Volume of each reactor
Ca0 = 10; %initial Ca (concentration of A species)
Cb0 = 0; %initial Cb (concentration of B species)
k = 0.9; %rate constant
kd = 0.01;%decay constant
tspan = 0:0.01:60; %time interval
y0 = [Ca0 0 0 1 1 1]; %initial concentrations of each reactor of A & initial values of catalyst activity
%differential equations
dydt=@(t,y)[(v0*Ca0-v0*y(1)-k*V*y(4)*y(1))/V;(v0*y(1)-v0*y(2)-k*V*y(5)*y(2))/V;(v0*y(2)-v0*y(3)-k*V*y(6)*y(3))/V;-kd*y(4);-kd*y(5);-kd*y(6)];
[t,y] = ode45(dydt,tspan,y0); %ode45 inbuilt method using to solve the differential equations
figure(1);
plot(t,y(:,1),'-',t,y(:,2),':',t,y(:,3),'--'); %plotting graph between Ca1 & t,  Ca2 & t, Ca3 wrt t
xlabel('Time(min)'), ylabel('Concentration(gmol/dm^3)')
legend('C_{A1}','C_{A2}','C_{A3}');
```

Results 1(A): -

Plot of concentration of A in each of the three reactors as a function of time to 60 mins



Solution 1 (B): -

Algorithm:-

- First we initialise all the parameters.
- Then since the activity coefficient depends on concentration of B we create an array y of size 9, where y(1), y(2) and y(3) store C_{A1}, C_{A2} and C_{A3} respectively and y(4), y(5) and y(6) store a_1 , a_2 and a_3 respectively, and y(7), y(8) and y(9) store C_{B1}, C_{B2} and C_{B3} respectively.
- Next we define the function dydt which returns a 1d array of size 9 whose i^{th} index stores the differential equation for i^{th} variable y(i).
- Then we use the built-in ode45 method for solving the system of ODEs.
- Finally we plot graphs of 1^{st}, 2^{nd} and 3^{rd} columns of y vs time where 1^{st} column stores values of C_{A1}, 2^{nd} column stores values of C_{A2} and third column stores values of C_{A3} respectively.

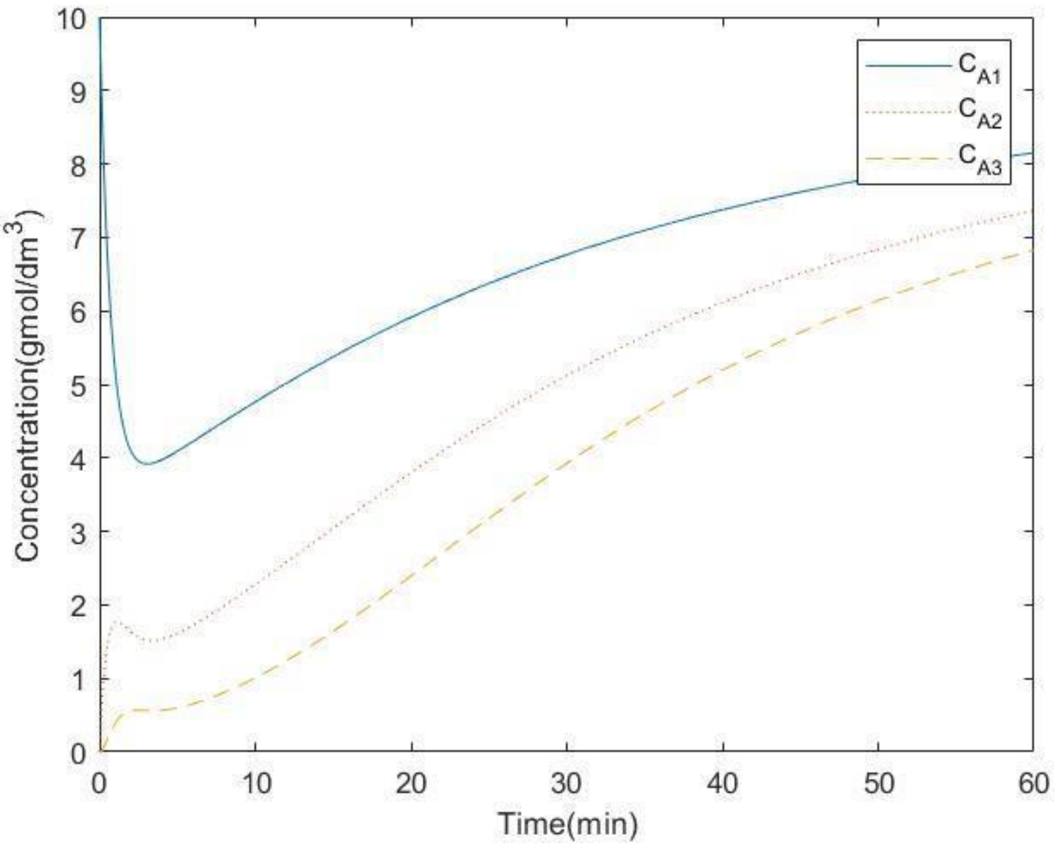
Code: -

```
v0 = 5; %inlet flow rate
V = 10; %Volume of each reactor
Ca0 = 10; %initial Ca (concentration of A species)
Cb0 = 0; %initial Cb (concentration of B species)
k = 0.9; %rate constant
```

```
kd = 0.01; %decay constant
tspan = 0:0.01:60;   %time interval
y0 = [Ca0 0 0 1 1 1 Cb0 0 0]; %initial concentrations of A & intial values of activity constants & initial values of concentrations of B.
%differential equations
dydt = @(t,y)[(v0*Ca0-v0*y(1)-k*V*y(4)*y(1))/V;(v0*y(1)-v0*y(2)-k*V*y(5)*y(2))/V;(v0*y(2)-v0*y(3)-k*V*y(6)*y(3))/V;-kd*y(4)*y(7);-kd*y(5)*y(8);-kd*y(6)*y(9);
 (v0*Cb0-v0*y(7)+k*V*y(4)*y(1))/V ; (v0*y(7)-v0*y(8)+k*V*y(5)*y(2))/V;(v0*y(8)-v0*y(9)+k*V*y(6)*y(3))/V];
[t,y] = ode45(dydt,tspan,y0); %ode45 inbuilt method using to solve the differential equations
figure(2);
plot(t,y(:,1),'-',t,y(:,2),':',t,y(:,3),'--'); %plotting graph between Ca1 & t,  Ca2 & t, Ca3 wrt t
xlabel('Time(min)'), ylabel('Concentration(gmol/dm^3)')
legend('C_{A1}','C_{A2}','C_{A3}');
```

Results 1(B): -

Plot of concentration of A in each of the three reactors as a function of time to 60 mins



Solution 2: Algorithm:-

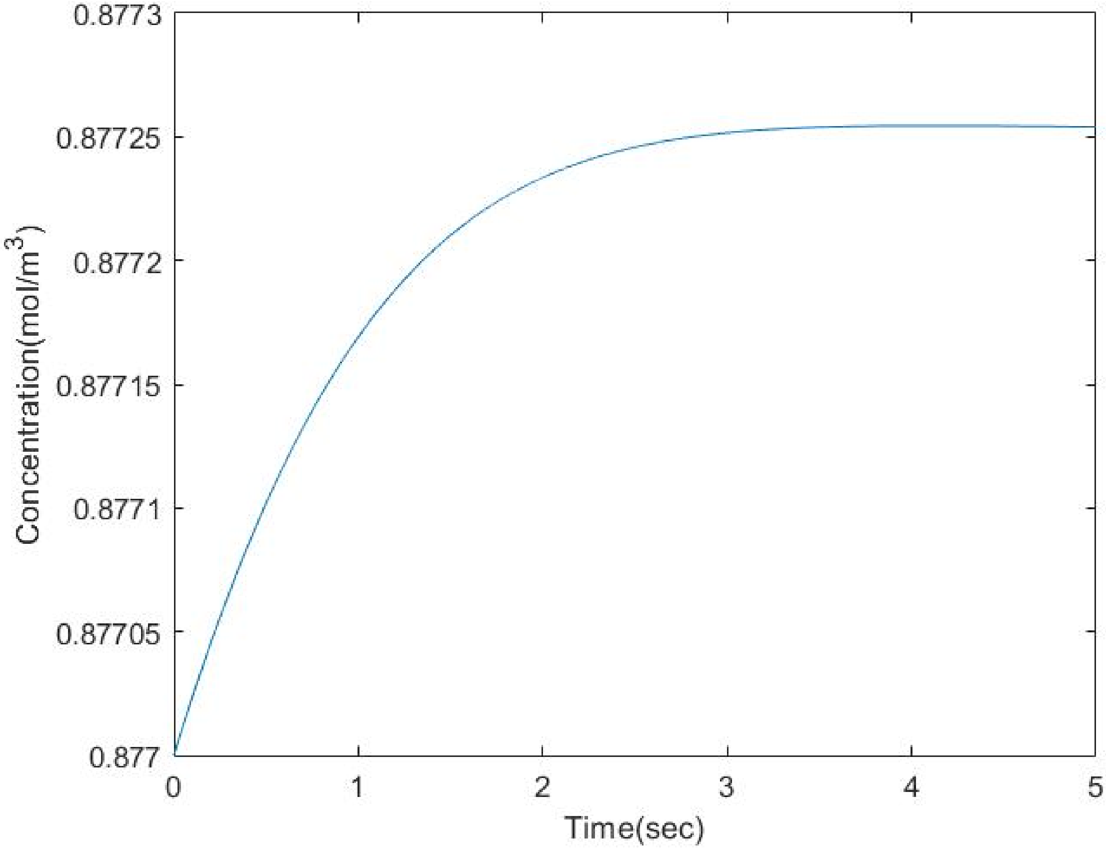
- First we initialise all the parameters.
- Then we create an array y of size 2 where y(1) stores concentration and y(2) stores temperature respectively.
- Next we define the function dydt which returns a 1d array of size 2 whose i^{th} index stores the differential equation for i^{th} variable y(i).
- Then we use the built-in ode45 method for solving the system of ODEs.
- Finally we plot graphs of 1^{st} and 2^{nd} columns of y vs time where 1^{st} column stores values of concentration and 2^{nd} column stores values of temperature.

Code: -

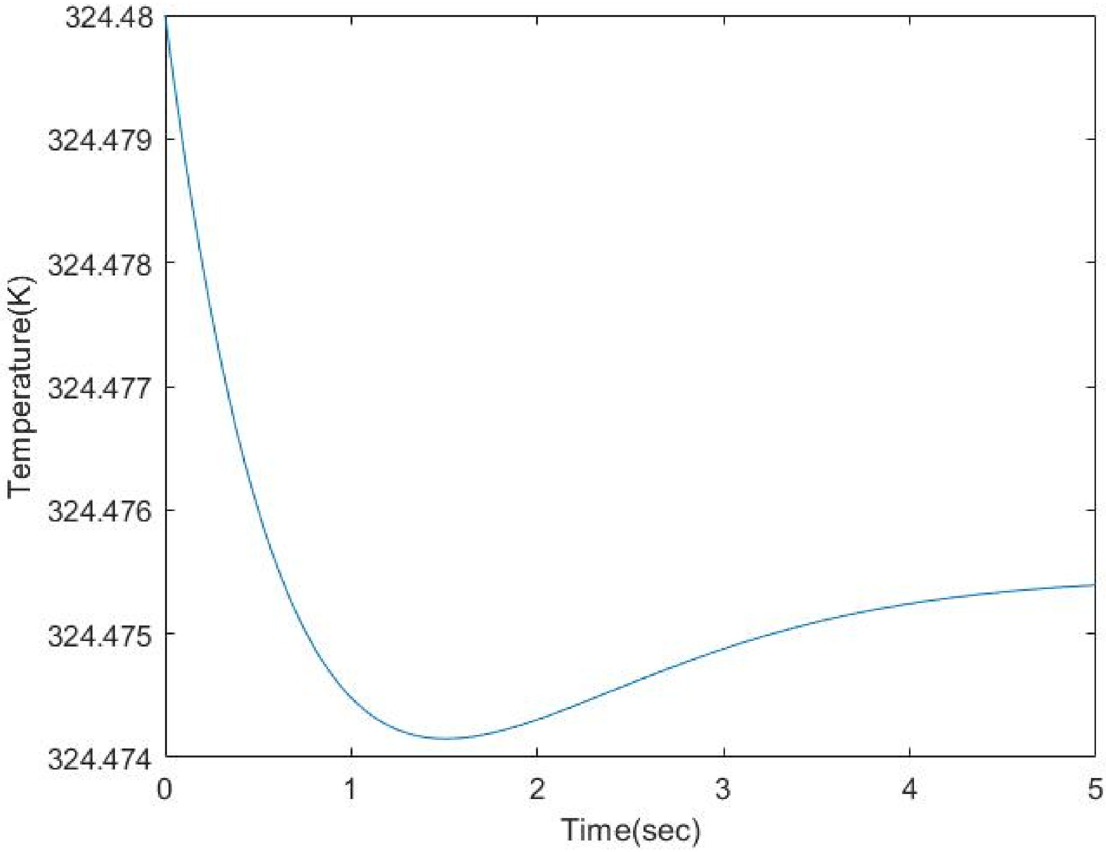
```
tspan = 0:0.001:5; %time_range
F = 100;%flow_rate
V = 100;%Volume of CSTR
CAf = 1;%Feed_concentration
alpha = 7.2e10;%pre_exponential_factor
E_R = 8750; %activation_energy/gas_constant
Tf = 350;%feed_temperature
delH = 5e4;%-1*heat_of_rxn
rho = 1000;%density of mixture
Cp = 0.239;% heat capacity of mixture
U_A = 50000;%overall_heat_transfer_coefficient
Tc = 300;%coolant_temperature
y0 = [0.877 324.48];%inital_concentration_and_initail_temperature
%differential_equations
dydt = @(t,y)[F/V*(CAf-y(1))-alpha*exp(-E_R/y(2))*y(1);
F/V*(Tf-y(2))+(delH/(rho*Cp))*alpha*exp(-E_R/y(2))*y(1)-
U_A/(V*Cp*rho)*(y(2)-Tc)];
[t,y] = ode45(dydt,tspan,y0);%solving_using_ode45
figure(3);
plot(t,y(:,1),'-')
xlabel('Time(sec)'), ylabel('Concentration(mol/m^3)')
figure(4);
plot(t,y(:,2),'-')
xlabel('Time(sec)'), ylabel('Temperature(K)')
```

Results of 2:-

Plots of concentration vs time and temperature vs time are as shown:-



0.8773
0.87725
0.8772
0.87715
0.8771
0.87705
0.877
Concentration(mol/m^3)
0
1
2
3
4
5
Time(sec)



324.48
324.479
324.478
324.477
324.476
324.475
324.474
Temperature(K)
0
1
2
3
4
5
Time(sec)