



Chemical Reactor Design Project

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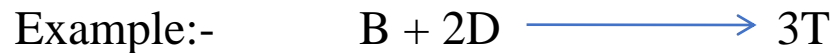
- **Reaction rate** :- Rate of a reaction is the rate at which reactant gets consumed or products are formed.



$$r(A) = -dC(A)/dt$$

$$-r(A)/a = -r(B)/b = r(C)/c = r(D)/d$$

- A reaction is either elementary or complex in nature.
- Elementary reaction is one which gets completed via a single step and whose rate can be written from stoichiometric coefficients whereas a complex reaction is one which takes more than one step for completion and its rate can be written only after thorough study of reaction steps.
- **Molecularity**:- Molecularity of a reaction is defined as the number of molecules that come together to react in an elementary reaction. Molecularity is always a positive integer and cannot be fractional or negative. It is always ≤ 3 .
- **Order** :- The order of reaction refers to the power dependence of the rate on the concentration of a single species. It can be positive, negative or fractional even.



$$\text{rate} = k \cdot C_D^2 \cdot C_B$$

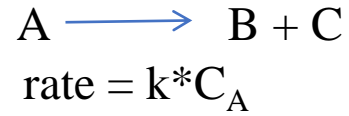
Here, overall order is $2+1 = 3$

- **Arrhenius Equation** :- $k_f = k_0 \exp(-E_a/RT)$
where k_0 is pre-exponential factor which accounts for effective number of collisions and E_a is the activation energy of the reaction.

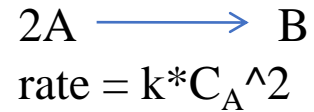




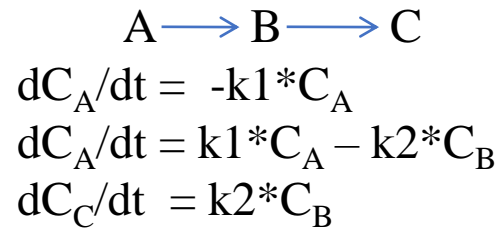
1st order Reaction :-



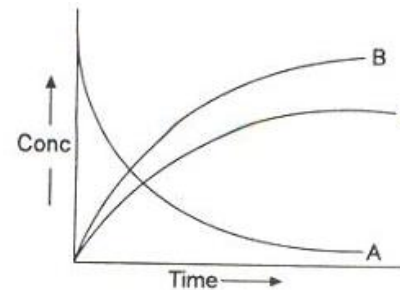
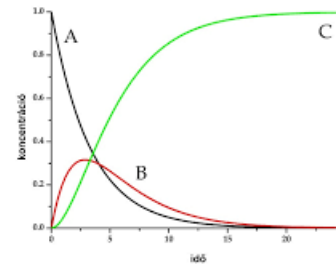
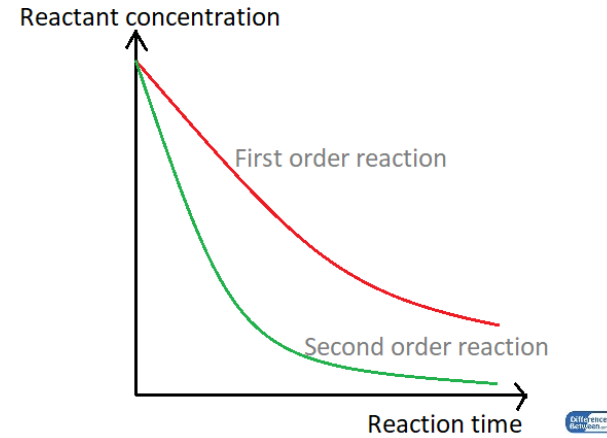
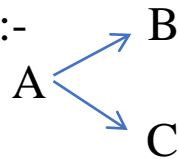
2nd order Reaction :-



Series Reactions :-



Parallel reactions :-





There are 4 types of reactors in general. These are:-

- Batch Reactor
- Semi-Batch Reactor
- Mixed flow reactor or CSTR
- Plug Flow Reactor (PFR)

Space Time :-

Time required to process one reactor volume of feed.

Space velocity:-

Number of reactor volume of feed that can be processed under specified condition.

Residence time:-

It is the time a fluid element actually remains within a reactor.





Batch Reactor

- A typical batch reactor consists of a storage tank and an agitator and integral heating/cooling system.
- They are usually fabricated in steel, stainless steel, glass-lined steel, glass or exotic alloy.
- A batch reactor is charged via two holes in the top of the tank, while reaction is carried out, nothing is put in or taken out.
- Concentration always changes with time and reactor is always at unsteady state.
- This reactor is suitable for all the three type of reactants and is used for small scale production.
- It is used widely in pharmaceutical industry.
- Its advantages are high conversion per unit volume for one pass and it is easy to clean.
- Its disadvantages include high operating cost and variable product quality.

■ Performance Equation:-

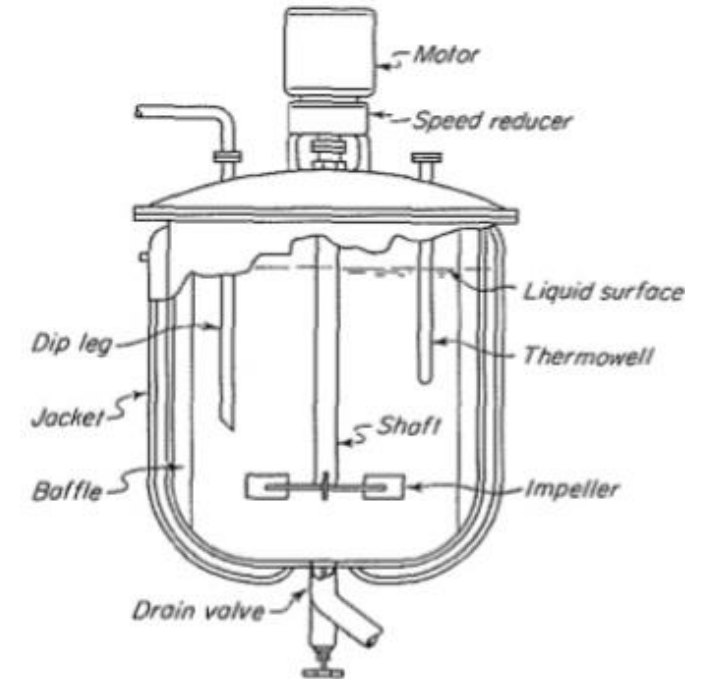
Material balance for batch reactor:-

input = output + disappearance by chemical reaction + accumulation

$$0 = 0 - r_A * V + dN(A)/dt$$

$$N_A = N_{A0} * (1 - X_A)$$

$$t = N_{A0} * \int dX_A / (-r_A * V)$$





Mixed Flow Reactor (MFR or CSTR)

- Similar to batch reactor in mechanical design, but has a continuous input/output.
- In a perfectly mixed reactor, reagent is instantaneously and uniformly mixed throughout the reactor upon entry. Consequently, the output composition is identical to composition of the material inside the reactor.
- This reactor is suitable for all the three types of reactants:- gases, liquids, and slurries.
- It is widely used as fermentors and bio-reactors.
- Its advantages are good temperature control and its behavior is very well understood.
- Its disadvantages include lower overall throughput per volume and not suitable for slow kinetics.

- **Performance Equation:-**

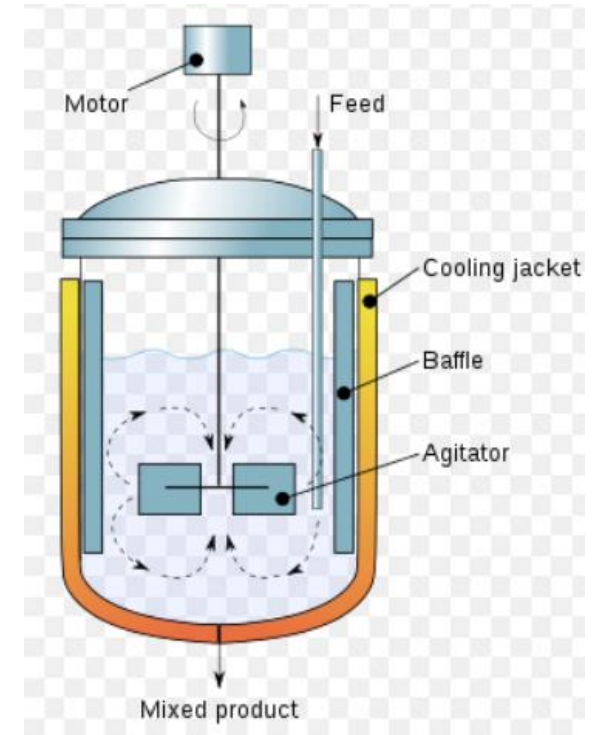
Material balance for MFR reactor:-

input = output + disappearance by chemical reaction + accumulation

$$F_{A0} = F_A - r_A * V + 0$$

$$F_A = F_{A0} * (1 - X_A)$$

$$V/F_{A0} = X_A / (-r_A)$$





Plug Flow Reactor (PFR)

- It is a long reactor tube or many short reactors in a tube bank and is used for continuous production.
- No mixing occurs in axial direction but there is infinite mixing in radial direction.
- This reactor is suitable for primarily gas phase and liquid phase only.
- It is widely used in gasoline production and oil cracking.
- Its advantages are high conversion per unit volume and good heat transfer.
- Its disadvantages include poor temperature control and undesired thermal gradients may exist.

- **Performance Equation:-**

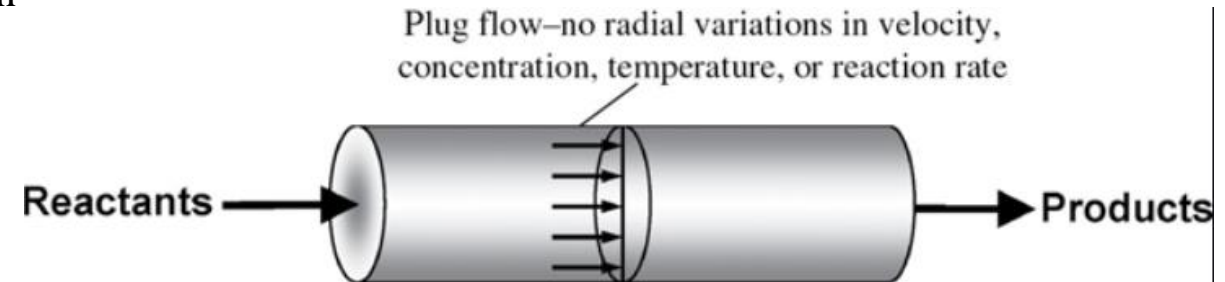
Material balance for PFR reactor:-

input = output + disappearance by chemical reaction + accumulation

$$F_A = F_A + dF_A - r_A * dV + 0$$

$$F_A = F_{A0} * (1 - X_A)$$

$$V/F_{A0} = \int dX_A / (-r_A)$$





General energy balance equation :-

$$dQ/dt - dW_s/dt + \sum F_{i0} * H_{i0} - \sum F_i * H_i = dE_{sys}/dt$$

Note:-

- Work done by the system is positive and work done on the system is negative.
- The above result equation is the result of energy balance performed on the whole reactor.

Now on simplifying some terms we get the final equation at steady state as:-

$$dQ/dt - dW_s/dt + F_{A0} \sum \Theta_i * C_{pi} * (T - T_0) - [\Delta H_{rxn}(T_R) + \Delta C_p (T - T_R)] * F_{A0} * X_A = 0$$

where $\Theta_i = F_{i0} / F_{A0}$ and T_0 is the inlet temperature.





Steady State CSTR with heat effects:-

Governing equations:-

- $F_{A0} * X_A = (-r_A) * V$
- $dQ/dt - dW_s/dt + F_{A0} \sum \Theta_i * C_{pi} * (T - T_0) - [\Delta H_{rxn}(T_R) + \Delta C_p (T - T_R)] * F_{A0} * X_A = 0$
- $dQ/dt = C_p * (T_{a1} - T_{a2}) * dm/dt = U * A * (T_{a1} - T_{a2}) / \ln((T - T_{a1}) / (T - T_{a2}))$

If X is specified, calculate T and V (design):-

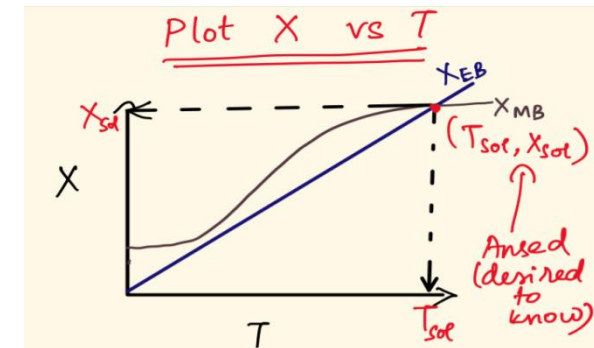
$$\text{Need } k=k(T) \longrightarrow T = \frac{F_{a0} * X_a (-H_{rxn}) + U * A * T_A + F_{a0} * C_{pa} * T_{a0}}{U * A + F_{a0} * C_{pa}} \longrightarrow V = \frac{(1 + \epsilon * X_A) * F_{a0} * X_A}{(k C_{a0}) * (1 - X_A)}$$

If V is specified, calculate T and X (simulation):-

$$X_{MB} = \frac{t * k}{(1 + k * t)} \longrightarrow X_{MB} = \frac{t * k_0 \exp(-E/R * T)}{(1 + k_0 \exp(-E/R * T))}$$

where $t = V * C_{A0} / F_{A0}$

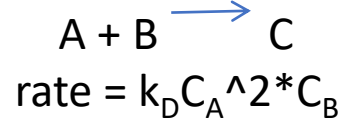
$$X_{EB} = \frac{(U * A * (T - T_0) / F_{A0} + C_{pA} * (T - T_0))}{[-\Delta H_{rxn}]}$$



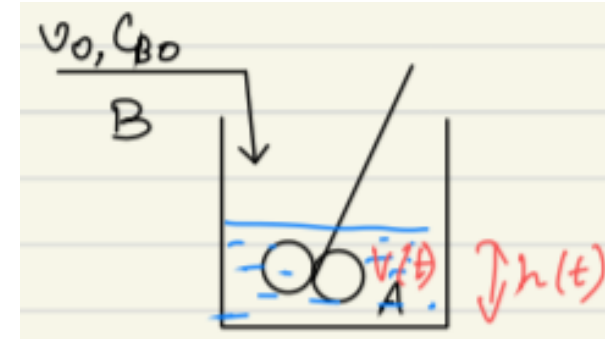
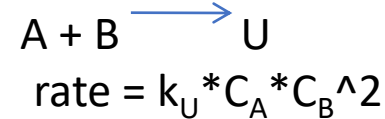


Special case:-

Desired Reaction:-



Undesired Reaction:-



Selectivity :- $S_{D/U} = k_D C_A / k_U C_B$

Note :- For selectivity to be high, we should keep C_A high and C_B low. So B is fed slowly to A in the vat.

Mole balance on A:-

Rate in – Rate out + Rate of Generation = Rate of Accumulation

$$0 - 0 + r_A * V = dN_A/dt$$

$$dC_A/dt = r_A - v_0 * C_A / V$$

Mole Balance on B:-

Rate in – Rate out + Rate of Generation = Rate of Accumulation

$$F_{B0} - 0 + r_B * V = dN_B/dt$$

$$dC_B/dt = r_B - v_0 * (C_B - C_{B0}) / V$$

where v_0 is volumetric flow rate and V is volume of reactor





Steady and simulate the concentration profile and temperature profile for an exothermic reaction w.r.t. time.

Esterification reaction:-



Data:-

$U=75$; $A=2.7414$; $\rho_{\text{Cp}}=53.25$; $V_r=0.4153$; $E_a=32400$; $H_{\text{rxn}}=-39000$; $k_0=16.96 \times (10^{12})$; $\rho_{\text{H}_2\text{O}}=1.001$; $C_{\text{pw}}=62.4$; $R=1.987$;
 $u_0=0.98$; $T_a=19.5$; $T_f=70$; $V_j=0.4746$;

For $t < 5$:- $C_{\text{af}}=0.132$; for $t \geq 5$:- $C_{\text{af}}= 1.5 \times 0.132$

- Do transient mole balance on CSTR, transient energy balance on CSTR and also on the cooling jacket to setup the differential equation.
- Use Matlab or any other software to solve the 3 differential equations and plot the evolution of concentration, temperature in the reactor as well as temperature of the coolant with time.
- Compare the result for different volumetric flow rate of coolant.
- After what time, the concentration, temperature in the reactor, and temperature of the coolant reaches steady state ?





Solution:-

Equations used:-

- **Mole Balance at unsteady state:-**

$$dN_A/dt = F_{A0} - F_A - V \cdot r_A$$

- **Energy Balance on Reactor:-**

$$dE/dt = U \cdot A \cdot (T_R - T_C) + \Delta H_{rxn} \cdot r_A \cdot V - \sum F_{i0} \cdot C_{pi} \cdot (T_R - T_i)$$

- **Energy Balance on Coolant Jacket:-**

$$dE/dt = U \cdot A \cdot (T_R - T_C) + u \cdot (T_a - T_c) \cdot C_{pw} \cdot \rho_w$$

Approach:-

The data given was stored in the variables. After this, an inbuilt function ode45 was used to simultaneously solve the 3 differential equations. Since the inlet concentration varies after 5 hrs, there are two sets of differential equations which needs to be solved. Therefore the values of the 3 variables namely the outlet temperature of the reactor, coolant and concentration of the reactant after 5 hrs was stored and used as initial conditions for the system of equations after 5hrs. As a result 6 graphs are produced from this simulation process.





```

U=75;
A=2.7414;
rho_Cp=53.25; %% rho*Cp for reactant
Vr=0.4153;
Ea=32400;
Hrxn=39000;
k0=16.96*(10^12);
rho_w=1.001;
Cpw=62.4;
R=1.987;
u0=0.98; %% volumetric flow rate
Caf1=0.132; %% will update Caf according to new question once code gets corrected
Caf2=1.5*0.132;
Ta=19.5;
Tf=70;
Vj=0.4746;
temp=zeros(5,3);
for u=0.5:1:5
f1=@(t,y)[U*A*(y(1)-y(3))/(rho_Cp*Vr)-y(2)*(Hrxn*k0)*exp(-(Ea)/(R*(y(1)+460)))/(rho_Cp)+u0*(Tf-y(1))/Vr;
y(2)*k0*Vr*exp(-Ea/(R*(y(1)+460)))/u0+Caf1/0.98-y(2)/u0;
U*A*(y(1)-y(3))/(rho_w*Cpw*Vj)+(u*(Ta-y(3)))/Vj];
[t1,y1] = ode45(f1,[0 5],[70 0 19.5]);
temp=y1;
%%[t2,y2] = ode45(f2,[5 10],[y1(5,1) y1(5,2) y1(5,3)]);
figure(1); %% outlet temp of reactor
plot(1*t1,y1(:,1));
xlabel("Time(hr)");
ylabel("Temperature of outlet (in F)");

figure(2); %% concentration wrt time
plot(1*t1,y1(:,2));
xlabel("Time(hr)");
ylabel("Concentration(lb-mol/ft^3)");

figure(3); %% outlet temperature of coolant
plot(1*t1,y1(:,3));
xlabel("Time(hr)");
ylabel("Temperature of coolant(in F)");
lgd=legend('0.5','1.5','2.5','3.5','4.5');
lgd.Title.String='Coolant Vol. Flow Rate(lb-mol/ft^3);
hold on;

f2=@(t,y)[U*A*(y(1)-y(3))/(rho_Cp*Vr)-y(2)*(Hrxn*k0)*exp(-(Ea)/(R*(y(1)+460)))/(rho_Cp)+u0*(Tf-y(1))/Vr;
y(2)*k0*Vr*exp(-Ea/(R*(y(1)+460)))/u0+Caf2/0.98-y(2)/u0;
U*A*(y(1)-y(3))/(rho_w*Cpw*Vj)+(u*(Ta-y(3)))/Vj];

[t2,y2] = ode45(f2,[5 10],[temp(length(y1),1) temp(length(y1),2) temp(length(y1),3)]);
figure(4); %% outlet temp of reactor
plot(1*t2,y2(:,1));
xlabel("Time(hr)");
ylabel("Temperature of outlet(in F)");

figure(5); %% concentration wrt time
plot(1*t2,y2(:,2));
xlabel("Time(hr)");
ylabel("Concentration(lb-mol/ft^3)");

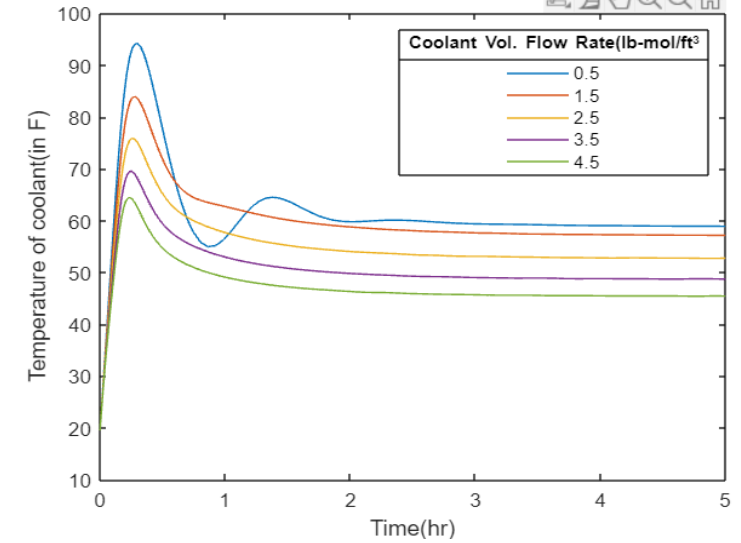
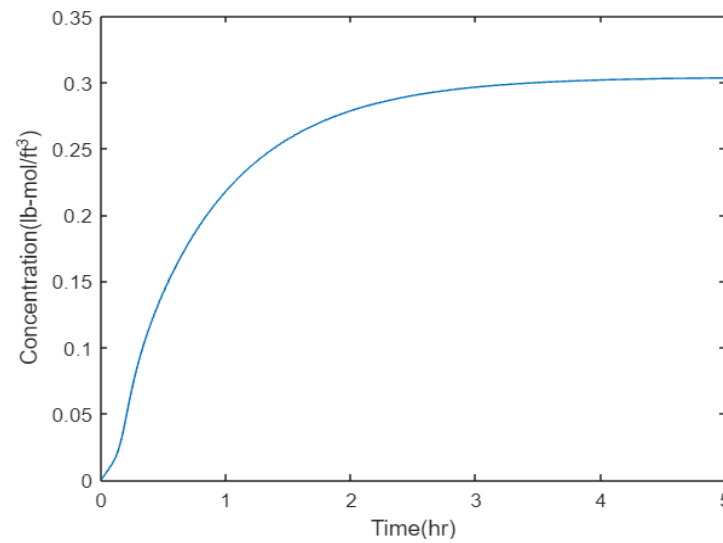
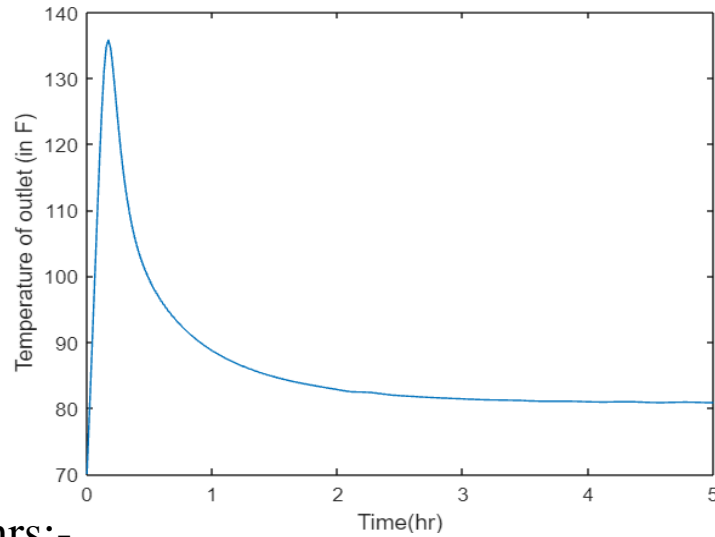
figure(6); %% outlet temperature of coolant
plot(1*t2,y2(:,3));
xlabel("Time(hr)");
ylabel("Temperature of coolant(in F)");

hold on;
end;

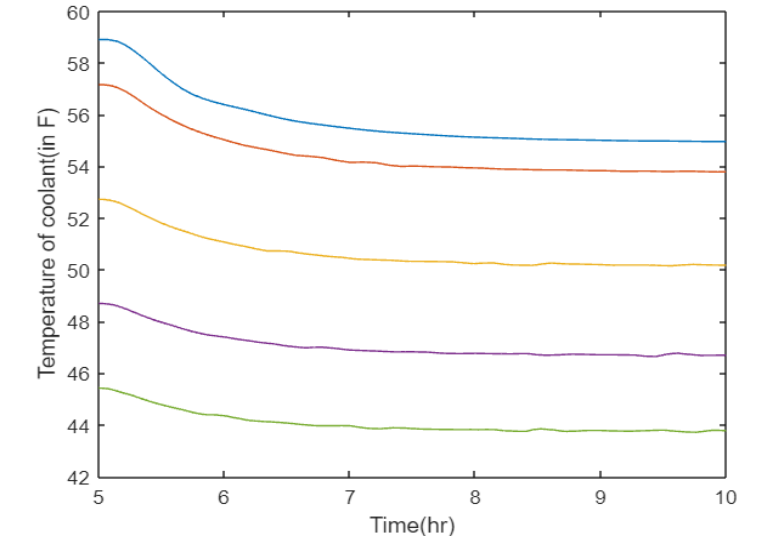
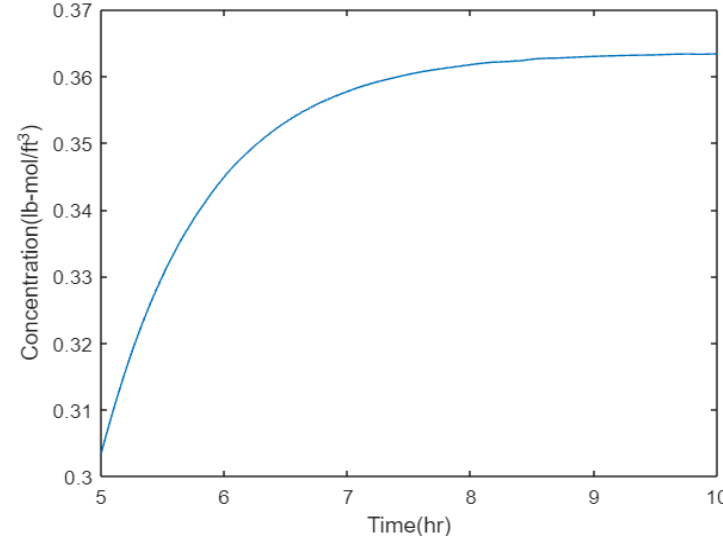
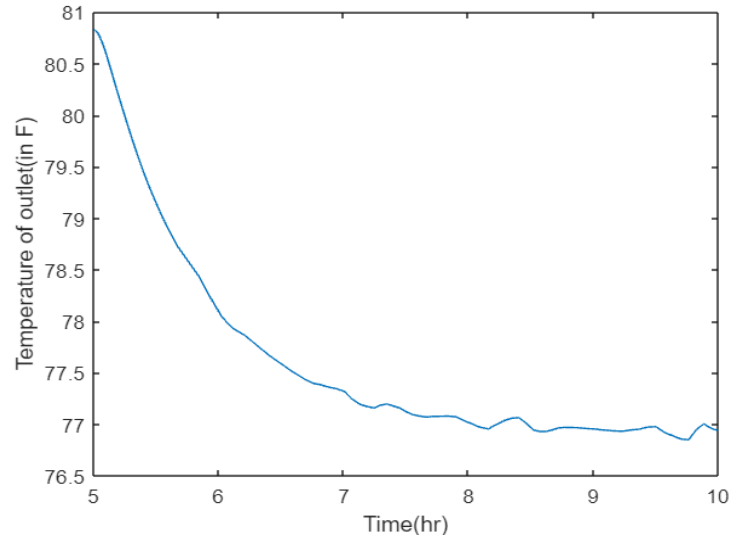
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For $t < 5$ hrs :-



For $t \geq 5$ hrs:-





Observations:-

- As evident from the first two figures the outlet temperature of the reactor starts from zero reaches a maximum and then becomes constant until the concentration of the reactant is further increased after 5 hrs and then finally the outlet temperature becomes constant at around 77 degree F.
- Next two figures show the concentration of the reactant inside the reactor. It is quite evident that the concentration increases and then becomes constant at about 0.3 lb-mol/ft³ until its concentration is increased and then finally becomes constant at higher value. This shows that the reactant first starts to accumulate and then its concentration becomes constant.
- The change in coolant volumetric flow rate has no impact on outlet temperature of reactor and concentration of reactant.
- As can be seen from figures 5 and 6, change in coolant volumetric flow rate has a significant impact over outlet temperature of coolant. The outlet limiting temperature of coolant is inversely proportional to its volumetric flow rate. On increasing the inlet concentration of reactant, the coolant temperature for each case further drops.





Conclusion:-

- For the given conditions in the question, change in volumetric flow rate has no effect on temperature of outlet and concentration of the reactant.
- Final temperature of both the outlet of the coolant and outlet of the reactor is greater than their respective inlet temperatures because the reaction of esterification is exothermic.
- After approximately 2hrs from the start of reaction, the outlet temperatures and concentration reaches their steady state but then after 5 hrs of completion, inlet concentration is changed which takes another 2-3 hrs to reach the final steady state and hence after about 8hrs the reaction reaches steady state.

