

```
%Variable Dictionary

%CA          Concentration of Methylcyclopentadiene
%CA0         Initial Concentration of Methylcyclopentadiene
%CB          Concentration of Sodium
%CB0         Initial Concentration of Sodium
%CS          Solvent Diglyme concentration
%CS0         Initial Solvent Diglyme concentration
%CD          Hydrogen Concentration
%CD0         Initial Hydrogen Concentration
%T           Temperature
%T_amb       Ambient Temperature
%T_crit      Critical Temperature
%P           Pressure
%P_crit      Critical Pressure
%t           Time
%t0          Initial Time
%t_max       Max Running Time of Batch Reactor
%t_span      Span of Time Reactor was running
%Vi          Volume of Liquid in Batch Reactor
%Vhead       Headspace Volume of Batch Reactor
%R_ideal     Ideal Gas Constant
%R_nonideal  Non-ideal Gas Constant
%Cv1         Specific Heat Capacity of Reaction 1
%Cv2         Specific Heat Capacity of Reaction 2
%SumNiCp     Sum of the Product of the Number of Moles of each Species
%k01 Rate    Equation pre-exponential factor for Reaction 1
%k02 Rate    Equation pre-exponential factor for Reaction 2
%Ea1         Activation Energy for Reaction 1
%Ea2         Activation Energy for Reaction 2
%Delt_H1     Enthalpy Change of Reaction 1
%Delt_H2     Enthalpy Change of Reaction 2
%UA_1        Cooling water for the Malfunctioning Reactor Scenario
%UA_2        Cooling water for the Functioning Reactor Scenario
%k1A         Rate Constant for Reaction 1
%k2S         Rate Constant for Reaction 2
%r1A         Rate of Reaction 1
%r2S         Rate of Reaction 2
%FD          Molar Flow Rate of Gas Leaving the Volume of Liquid
%Fvent       Molar Flowrate Out of the Reactor
%t_expl      Time when reactor explodes
%t_finish    Time at the End of the Reaction
%t_finish_mins Time at the End of the Reaction in Minutes

%Question 2A
clear all
clc

global CA CB CS CD T P Vi Vhead T_amb T_crit P_crit R_ideal...
      R_nonideal Cv1 Cv2 SumNiCp k01 Ea1 Delt_H1 k02 Ea2...
      Delt_H2 UA t
```

```

%Conditions within Batch Reactor
Vi = 4000; % L
Vhead = 5000; % L
T_amb = 373; % K
T_crit = 600; % K
P_crit = 45; % Atm
R_ideal = 8.314; % J / (mol K)
R_nonideal = 0.082; % J / (mol K)
Cv1 = 3360; % mol / (hr atm)
Cv2 = 53600; % mol / (hr atm)
SumNiCp = 1.26e+7; % J / K

%Reaction 1 variables
k01 = 4e+14; %L / (mol hr)
Ea1 = 128000; %J / mol
Delt_H1 = -45400; %J / mol

%Reaction 2 variables
k02 = 1e+84; %L / (mol hr)
Ea2 = 800000; %J / mol
Delt_H2 = -3.2e+5; %J / mol

%No cooling water is available in scenario for question 2a
UA = 0; % J / (hr K)

%Initial conditions for the reaction ODES
CA0 = 4.3; % mol / L
CB0 = 5.1; % mol / L
CS0 = 3; % mol / L
CD0 = 0; % mol / L
T0 = 422; % mol / L
P0 = 4.4; % mol / L

%Initial conditions converted to vector form
y0(1) = CA0;
y0(2) = CB0;
y0(3) = CS0;
y0(4) = T0;
y0(5) = P0;

%The length of time the ODEs will be plotted for
t0 = 0; % hrs
t_max = 4; % hrs
tspan = [t0,t_max]; % hrs

%The ODE function is called
[t,y] = ode15s(@t_explsn,tspan,y0);

CA = y(:,1);
CB = y(:,2);
CS = y(:,3);
T = y(:,4);
P = y(:,5);
%Equation for the behaviour of the Hydrogen gas in the Headspace Volume

```

```

CD = P/(R_nonideal*T);
%Plotting the graphs for the malfunctioning cooling system
plot(t,CA,'b-',t,CB,'m-',t,CS,'r-',t,CD,'k-')
xlabel('Time(hrs)');
ylabel('Concentration(mol/L)');
title('Concentration vs time graph for batch reactor');
legend('CA','CB','CS','CD')

```

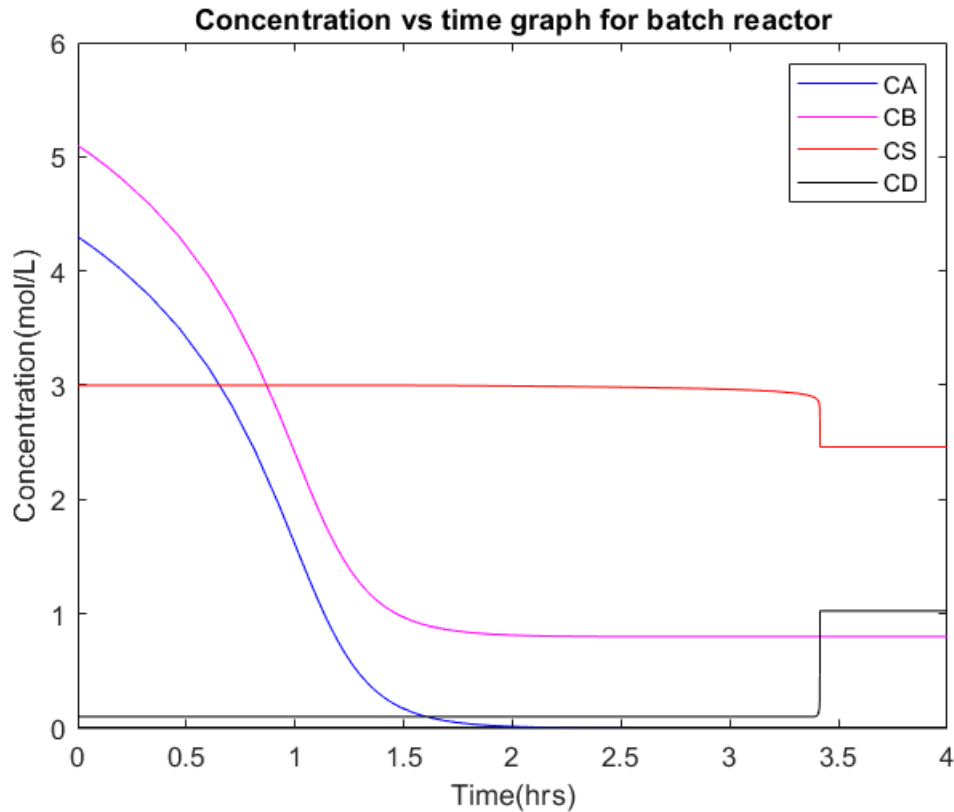


Figure 1: Graph for Concentration of the Substances with Respect to Time with Malfunctioning Cooling System

When looking at Figure 1, we can see that after maintaining a stable concentration there is a sudden drop in the concentration of Diglyme at around 3.4 hours, This shows that the Diglyme has started to decompose and produce hydrogen gas in the headspace volume in the process. Correspondingly the concentration of the Hydrogen in the headspace also increases, this leads to the sudden increase in pressure in the headspace of the batch reactor at the same time as can be seen in Figure 3. After the explosion of the batch reactor, it can be see that the concentration of diglyme remains constant again at around 2.5 mol/L, after dropping instantaneously from 3 mol/L.

```

plot(t,T)
xlabel('Time(hrs)');
ylabel('Temperature(K)');
title('Temperature vs time graph for batch reactor');

```

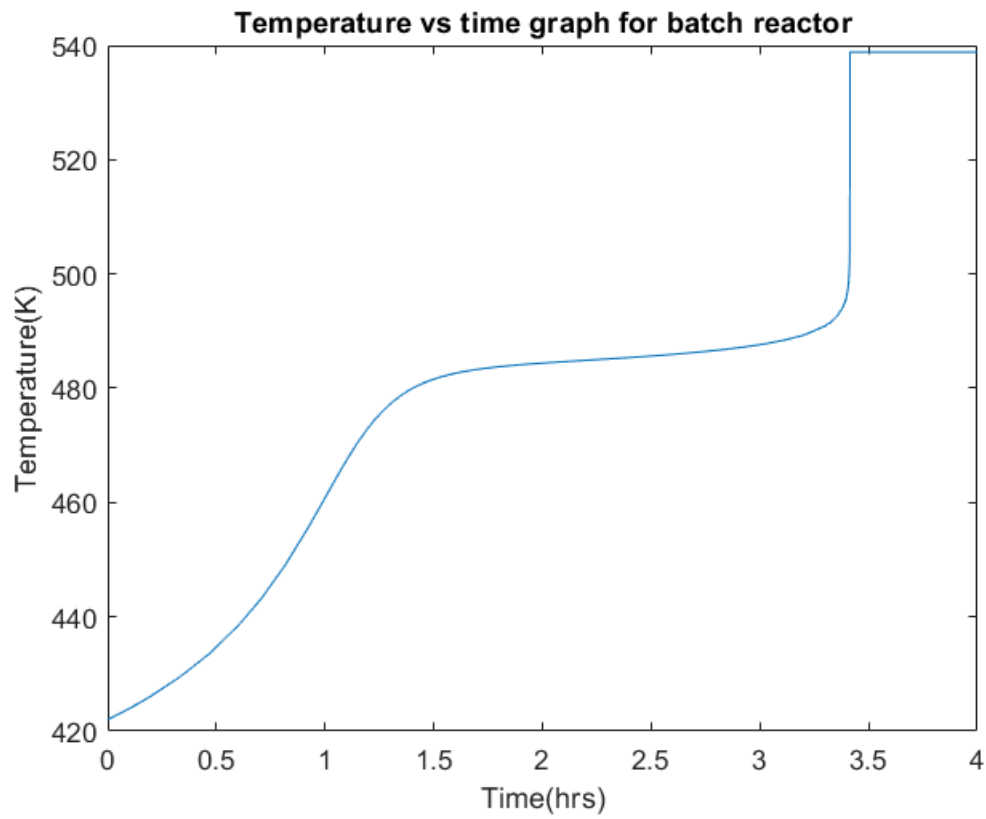


Figure 2: Temperature with Respect to Time with Malfunctioning Cooling System

```
plot(t,P)
xlabel('Time(hrs)');
ylabel('Pressure(atm)');
title('Headspace Pressure vs time graph for batch reactor');
```

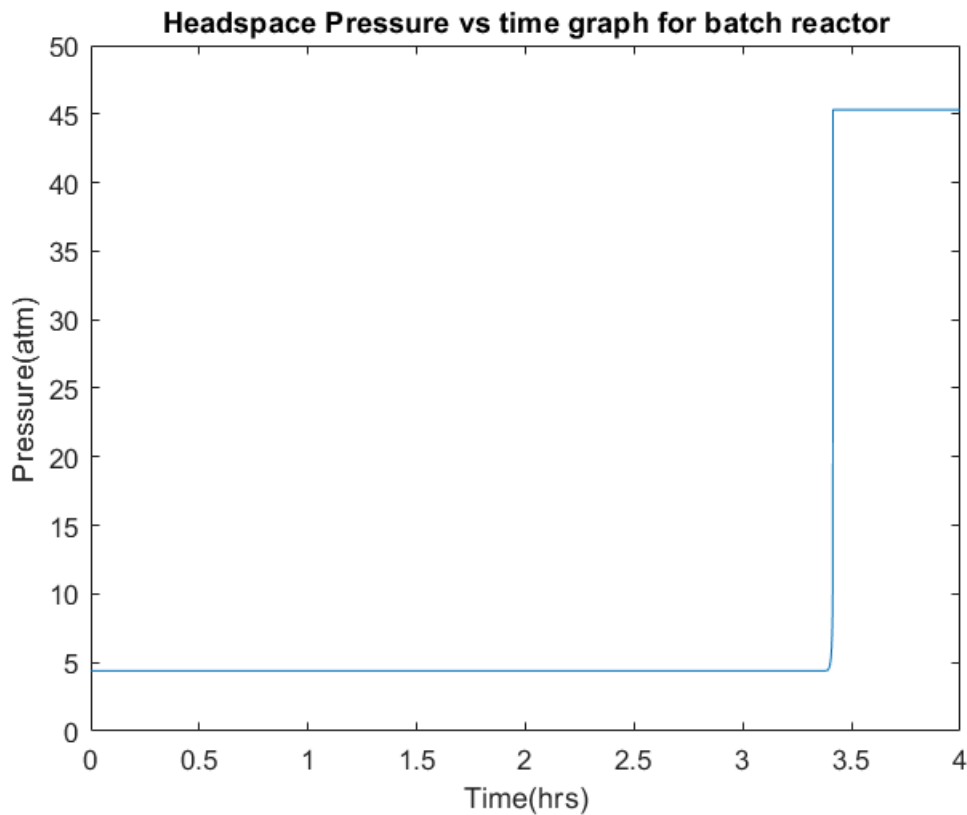


Figure 3: Headspace Pressure with Respect to Time with Malfunctioning Cooling System

#### %Question 2B

```

global UA
y0(1) = CA0;
y0(2) = CB0;
y0(3) = CS0;
y0(4) = T0;
y0(5) = P0;
%The length of time the ODEs will be plotted for
t0 = 0;
t_max = 4;
tspan = [t0,t_max];
%Our new cooling water value when batch reactor is fully operational
UA = 2.77e+6;
%Calling the same ODE as used in 2A
[t,y] = ode15s(@t_explsn,tspan,y0);

CA = y(:,1);
CB = y(:,2);
CS = y(:,3);
T = y(:,4);
P = y(:,5);
%Equation for the behaviour of the Hydrogen gas in the Headspace Volume
CD = P/(R_nonideal*T);

plot(t,CA, 'b-',t,CB, 'm-',t,CS, 'r-',t,CD, 'k-')

```

```

xlabel('Time(hrs)');
ylabel('Concentration(mol/L)');
title('Concentration vs time graph for batch reactor');
legend('CA', 'CB', 'CS', 'CD')
hold off

```

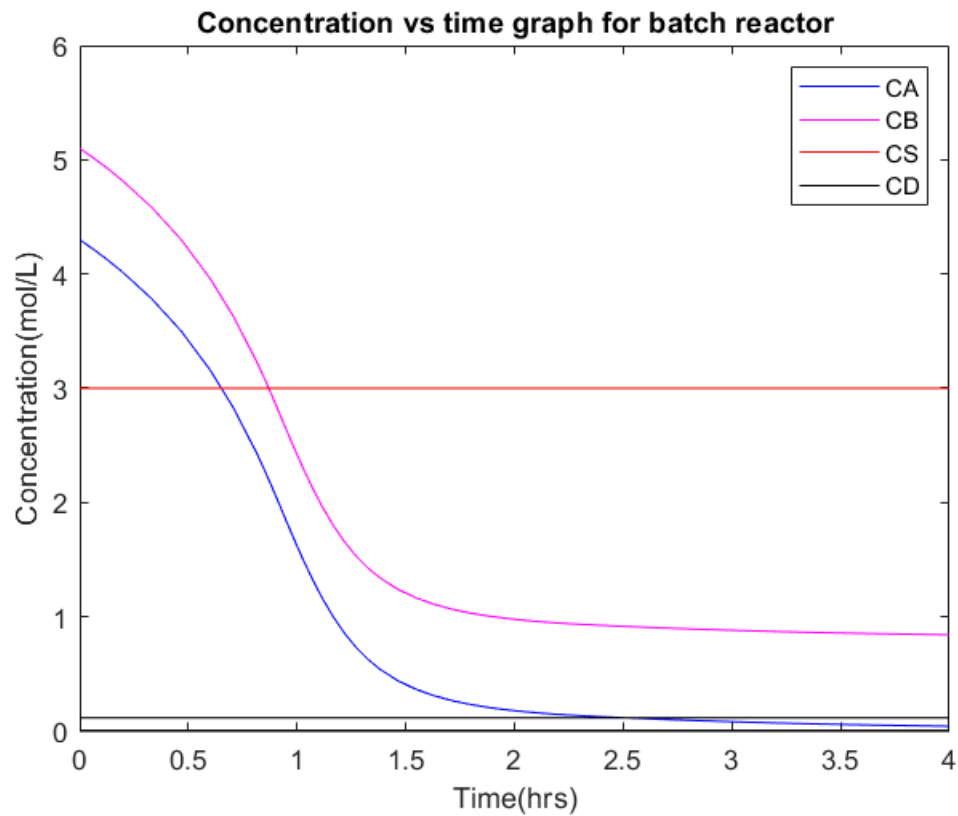


Figure 4: Graph for Concentration of the Substances with Respect to Time with Functioning Cooling System

```

plot(t,T)
xlabel('Time(hrs)');
ylabel('Temperature(K)');
title('Temperature vs time graph for batch reactor');
hold off

```

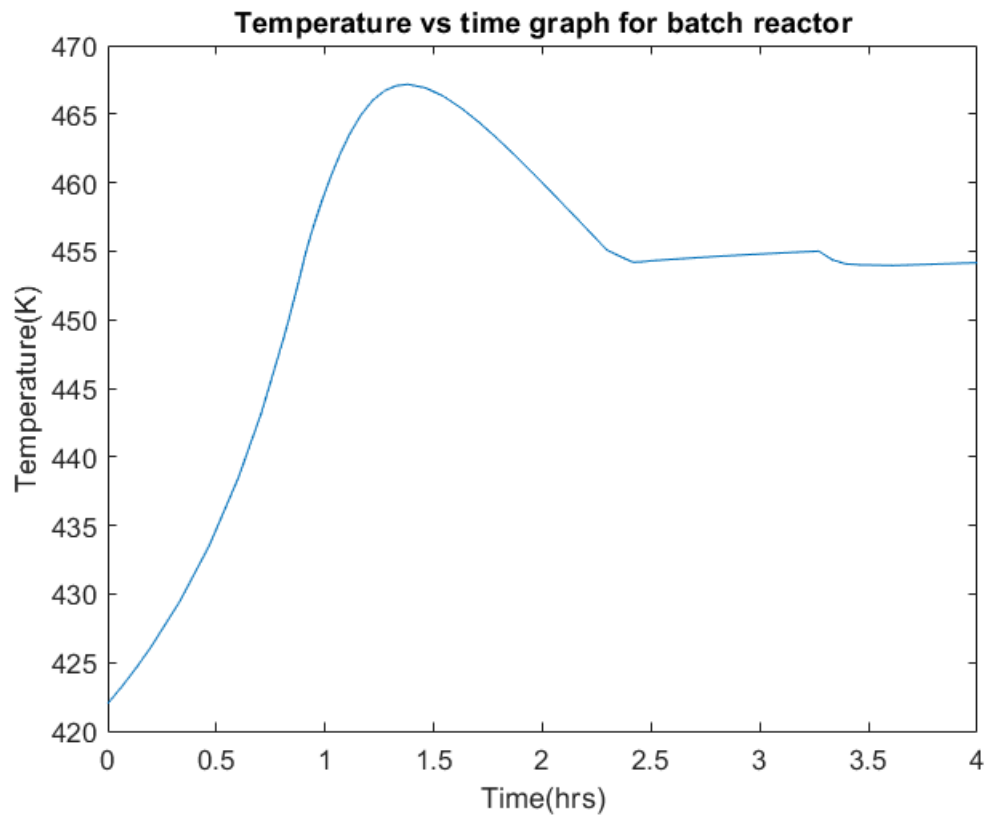


Figure 5: Temperature with Respect to Time with Functioning Cooling System

```
plot(t,P)
xlabel('Time(hrs)');
ylabel('Pressure(atm)');
title('Pressure vs time graph for batch reactor');
hold off
```

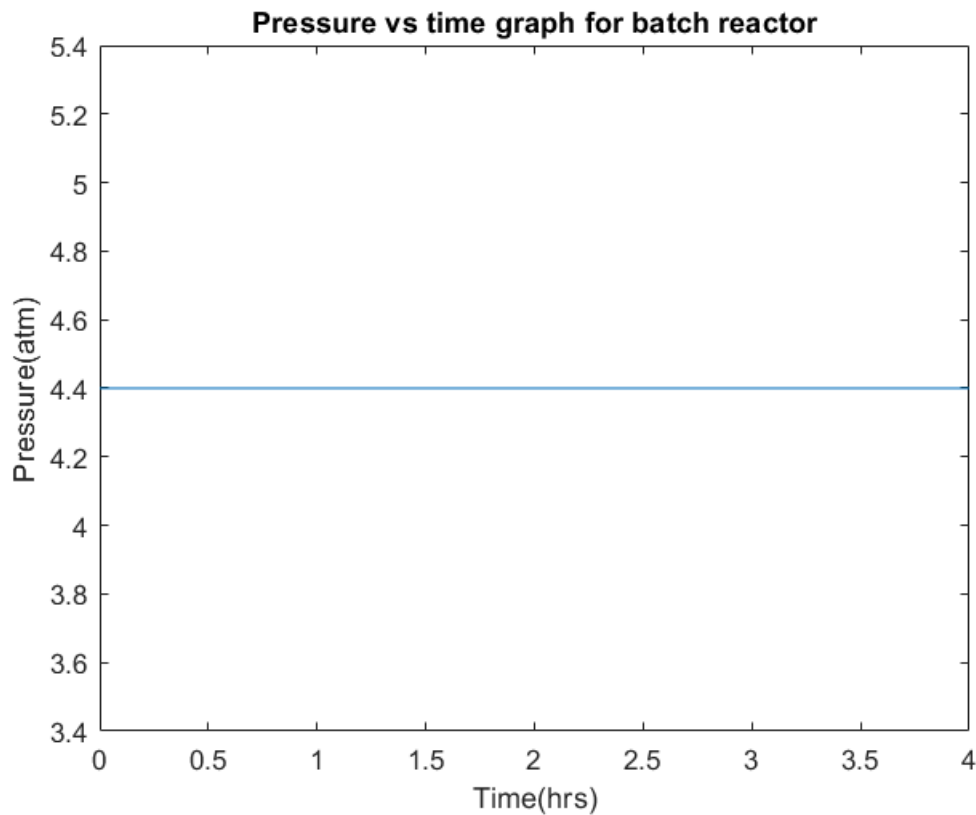


Figure 6: Headspace Pressure with Respect to Time with Functioning Cooling System

```
%Question 2C
global m t_activation
%Calling the ODE for Question 2C
[t,y] = ode15s(@Func2C,tspan,y0);

T_crit = y(:,1);
P_crit = y(:,2);

while max(T_crit,[]),'all' < T_explode && max(P_crit,[],'all') < P_explode

    m = m + 0.01;

    [t,y] = ode15s(@Func2C,tspan,y0);

    T_crit = y(:,1);
    P_crit = y(:,2);

end
```

Error using max  
Matrix dimensions must agree.

```
t_activation = (m - 0.01)*60;

fprintf(num2str(t_activation),('is the maximum amount of time to activate cooling water on the
```



## Question 2D

Larger diameter for the vent pipe:

The larger diameter will provide for more hydrogen gas in the batch reactor headspace to be removed, meaning that this will lead to less accumulation of the gas within the headspace and ultimately decrease the overall pressure within the headspace, therefore, inherently lowering the probability of a build-up of pressure and an explosion. The way this will work is that the greater diameter in the vent pipe will lead to a greater flow rate, due to the continuity principle of fluid mechanics ( $G = uA$ ), therefore a greater flowrate of the hydrogen gas produced being removed from the headspace, will lead to less accumulation of gas.

Smaller Batch Size:

The smaller batch size will ultimately lead to use of fewer amounts of the components with the reactions that occur within the reactor. The moles of each substance used within this smaller batch reactor will be lower compared to the original reactor, therefore the scale of the reaction will be smaller and less thermal energy will be released in the process. Less thermal energy being released means that less pressure will be built up in the reactor as the 2 are directly proportional to each other. Again, the less pressure build up will lead to a lower probability of it exceeding to a dangerous threshold where the reactor could potentially explode.

Larger headspace volume relative to liquid in the tank:

The larger headspace volume will mean that there is a greater volume for the hydrogen gas will accumulate in, this larger volume will mean that the hydrogen gas molecules will be further apart from each other in this volume, meaning that there will be less build up of pressure. Another way to accomplish this could be to use less liquid volume within the batch reactors already in use so that in the total volume, the vast majority of the volume is headspace volume.

Function for 2A and 2B

```
function dydt = t_explsn(t,y)
global t_explode t_finish_mins k1A k2S r1A r2S P P_crit FD Fvent...
k01 k02 Ea1 Ea2 R_ideal R_nonideal T T_amb T_crit Delt_H1 Delt_H2 ...
UA SumNiCp Vi Cv1 Cv2 Vhead CA CB CS t_finish

CA= y(1);
CB = y(2);
CS = y(3);
T = y(4);
P = y(5);

% Define Reaction Rate Constants
k1A = k01 * exp((-Ea1)/(R_ideal * T));
k2S = k02 * exp((-Ea2)/(R_ideal * T));
% Define reaction rate
r1A = - (k1A) * y(1) * y(2);
r2S = - (k2S) * y(3);

% Mole Balances
dCAdt = r1A;
```

```

dCBdt = r1A;
dCSdt = r2S;

% Temperature ODE Scenarios
if T >= 455 % K
    dTdt = (((Vi) .* ((r1A * Delt_H1) + (r2S * Delt_H2)) - (UA * (T - T_amb)))) ./ (SumNiCp));
else
    dTdt = (((Vi) .* ((r1A * Delt_H1) + (r2S * Delt_H2))) ./ (SumNiCp));
end

% Pressure ODE Scenarios
FD = (((-0.5 * r1A) - (3 * r2S)) * Vi);
%Conditions for which Fvent values will be used in the Pressure ODE
if FD < 11400 % mol/h
    Fvent = FD;
elseif FD > 11400 && P < 28.2 % atm
    Fvent = ((P - 1) .* (Cv1));
elseif FD > 11400 && P > 28.2 % atm
    Fvent = ((P - 1) .* (Cv1 + Cv2));
end

% Hydrogen model (Ideal Gas)
dPdt = ((FD - Fvent) .* (R_nonideal * T) ./ Vhead);

dydt(1) = dCAdt;
dydt(2) = dCBdt;
dydt(3) = dCSdt;
dydt(4) = dTdt;
dydt(5) = dPdt;

dydt = dydt';

if T >= T_crit || P >= P_crit
    dydt = 0;
while t_explode == 0
    t_finish = t;
    t_finish_mins = t_finish * 60;
    t_explode = 1;
    fprintf(['The reactor exploded at time, t = %.2f minutes.'],t_finish_mins)
end
end
end

```

Function for 2C

```

function dydt = Func2C(t,y)
global k1A k2S r1A r2S P P_crit FD Fvent...
k01 k02 Ea1 Ea2 R_ideal R_nonideal T T_amb T_crit Delt_H1 Delt_H2 ...
UA SumNiCp Vi Cv1 Cv2 Vhead CA CB CS m

CA= y(1);
CB = y(2);
CS = y(3);

```

```

T = y(4);
P = y(5);

% Define Reaction Rate Constants
k1A = k01 * exp((-Ea1)/(R_ideal * T));
k2S = k02 * exp((-Ea2)/(R_ideal * T));
% Define reaction rate
r1A = - (k1A) * y(1) * y(2);
r2S = - (k2S) * y(3);

% Mole Balances
dCA dt = r1A;
dCB dt = r1A;
dCS dt = r2S;

% Temperature ODE Scenarios
if T >= m
    dT dt = (((Vi) .* ((r1A * Delt_H1) + (r2S * Delt_H2)) - (UA * (T - T_amb)))) ./ (SumNiCp));
else
    dT dt = (((Vi) .* ((r1A * Delt_H1) + (r2S * Delt_H2))) ./ (SumNiCp));
end

% Pressure ODE Scenarios
FD = (((-0.5 * r1A) - (3 * r2S)) * Vi);

if FD < 11400 % mol/h
    Fvent = FD;
elseif FD > 11400 && P < 28.2 % atm
    Fvent = ((P - 1) .* (Cv1));
elseif FD > 11400 && P > 28.2 % atm
    Fvent = ((P - 1) .* (Cv1 + Cv2));
end

% Hydrogen model (Ideal Gas)
dP dt = ((FD - Fvent) .* (R_nonideal * T) ./ Vhead);

dydt(1) = dCA dt;
dydt(2) = dCB dt;
dydt(3) = dCS dt;
dydt(4) = dT dt;
dydt(5) = dP dt;

dydt = dydt';

if T >= T_crit || P >= P_crit
    dydt = 0;
end
end

```