

```

clear
clc
% defining general variables
V_ac = 210; %in ml, acetic acid
V_but = 340; %in ml, butanol
rho_ac = 1.05; %in g/ml
rho_but = 0.81; %in g/ml
M_ac = 60; % Molar mass
M_but = 74;
n_ac = (V_ac*rho_ac)/M_ac; % no. of moles
n_but = (V_but*rho_but)/M_but;
t = (0:10:80);

%For reactor 1:
T_r1 = [100, 100.2, 104, 113.5, 120.1, 123.4, 123.9, 124.2, 124.7];
V_naoh_r1 = [9.1, 8, 7.4, 6.3, 5.0, 4.3, 2.2, 1.2, 0.5]; %in ml
n_acid_r1 = 1*V_naoh_r1/1000; %mol of acid in sample neutralised by 1N NaOH
V_sample = 2; %volume of sample in ml
conc_acid_r1 = n_acid_r1*1000/V_sample;
cum_sample = (2:2:18);
water_lost = [0, 16.5, 15, 16, 11.5, 9.5, 5, 2.0, 1.3] ;%
cum_water_rem_r1 = zeros(1, length(water_lost));
for i=2:9
    cum_water_rem_r1(i) = water_lost(i)+cum_water_rem_r1(i-1);
end
vol_in_r1 = 550-cum_sample-cum_water_rem_r1;
n_acid_reacted_r1 = (vol_in_r1.*conc_acid_r1)/1000;
X1 = (n_ac-n_acid_reacted_r1)/(n_ac);

```

```

X1 = 1×9
    0.3215    0.4237    0.4840    0.5761    0.6728    0.7253    0.8616    0.9251 ...

```

```

V_W_naoh = [0, 9, 7.1, 6.1, 5.1, 4.1, 4.4, 2.4, 1.5];
V_W = 5; % ml

```

```

V_W = 5

```

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acid_lost = ((1.*V_W_naoh)) % in millimoles

```

```

acid_lost = 1×9
    0    9.0000    7.1000    6.1000    5.1000    4.1000    4.4000    2.4000 ...

```

```

total_acid_lost=sum(acid_lost)

```

```

total_acid_lost = 39.7000

```

```

%For reactor 2:
T_r2 = [98.7, 97.4, 97, 96.9, 96.4, 96.5, 96.5, 96.6, 96.5];
V_naoh_r2 = [9.5, 8.5, 7.2, 6.2, 5.5, 5, 4.6, 4.4, 4.6];
n_acid_r2 = 1*V_naoh_r2/1000;
conc_acid_r2 = n_acid_r2*1000/V_sample;
V_in_r2 = 550-cum_sample;

```

```
n_acid_reacted_r2 = (V_in_r2.*conc_acid_r2)/1000;
X2 = (n_ac-n_acid_reacted_r2)/n_ac;
```

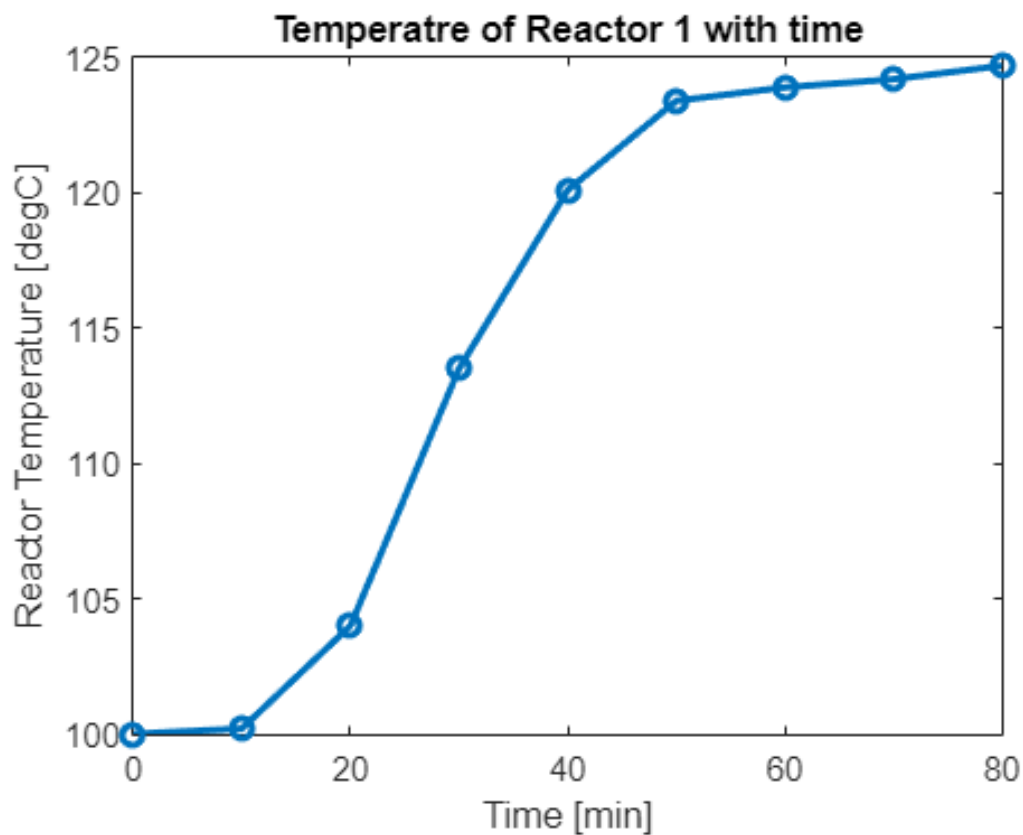
```
%Enhancement factor:
```

```
E = (X1-X2)./X2;
```

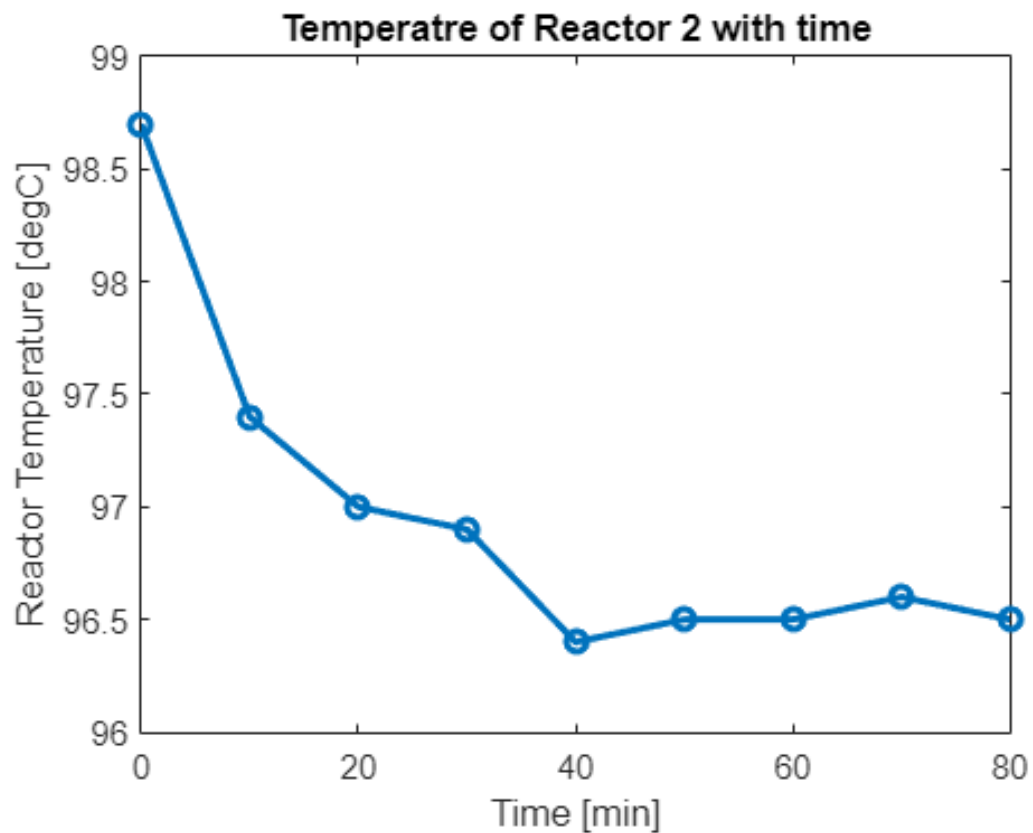
```
% error analysis
```

```
%Plots
```

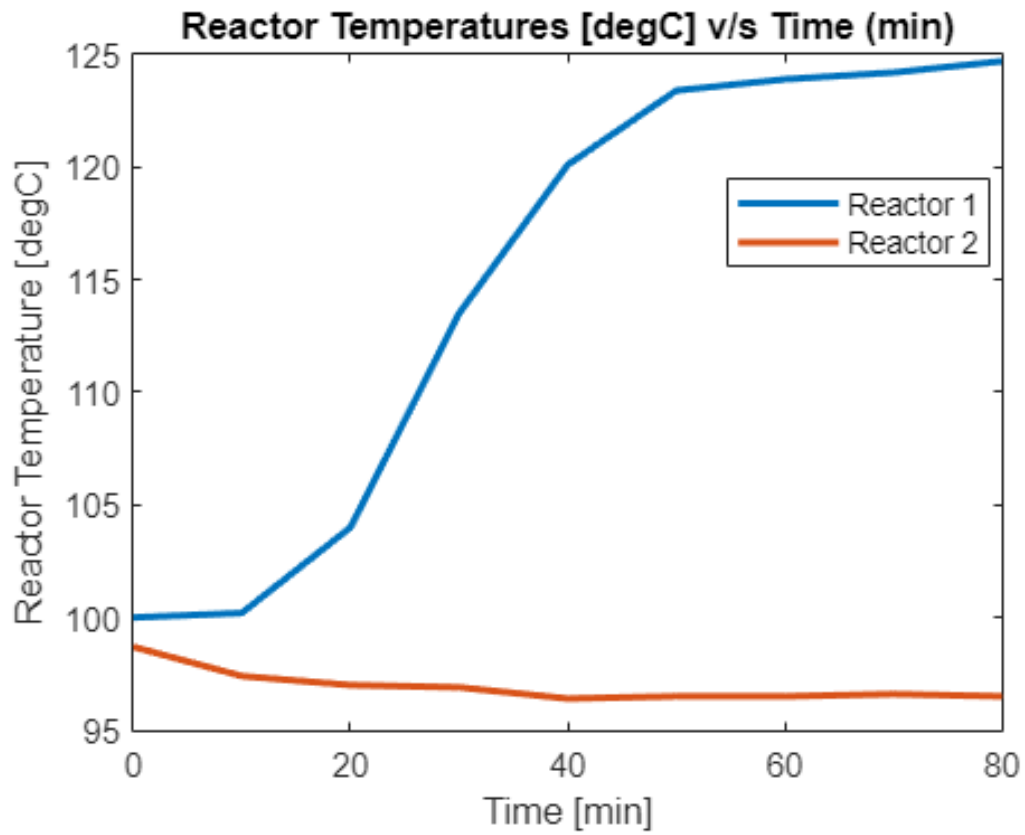
```
plot(t, T_r1, '-o', 'LineWidth', 2)
title('Temperatre of Reactor 1 with time')
ylabel('Reactor Temperature [degC]')
xlabel('Time [min]')
```



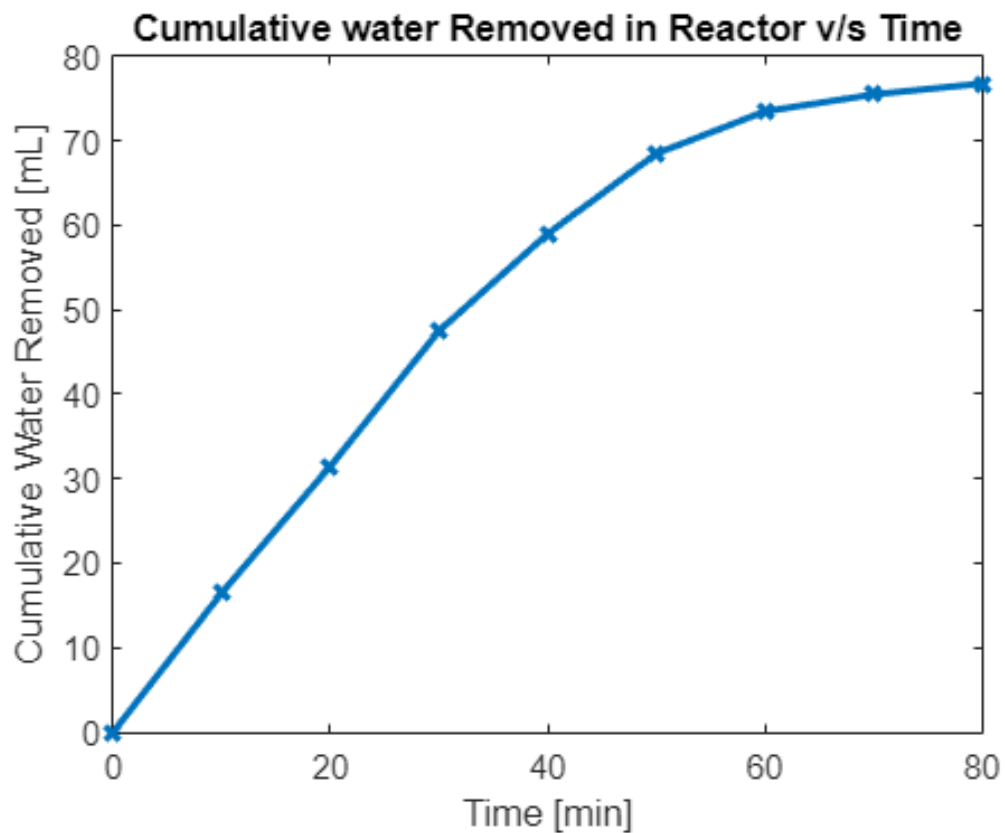
```
plot(t, T_r2, '-o', 'LineWidth', 2)
title('Temperatre of Reactor 2 with time')
ylabel('Reactor Temperature [degC]')
xlabel('Time [min]')
```



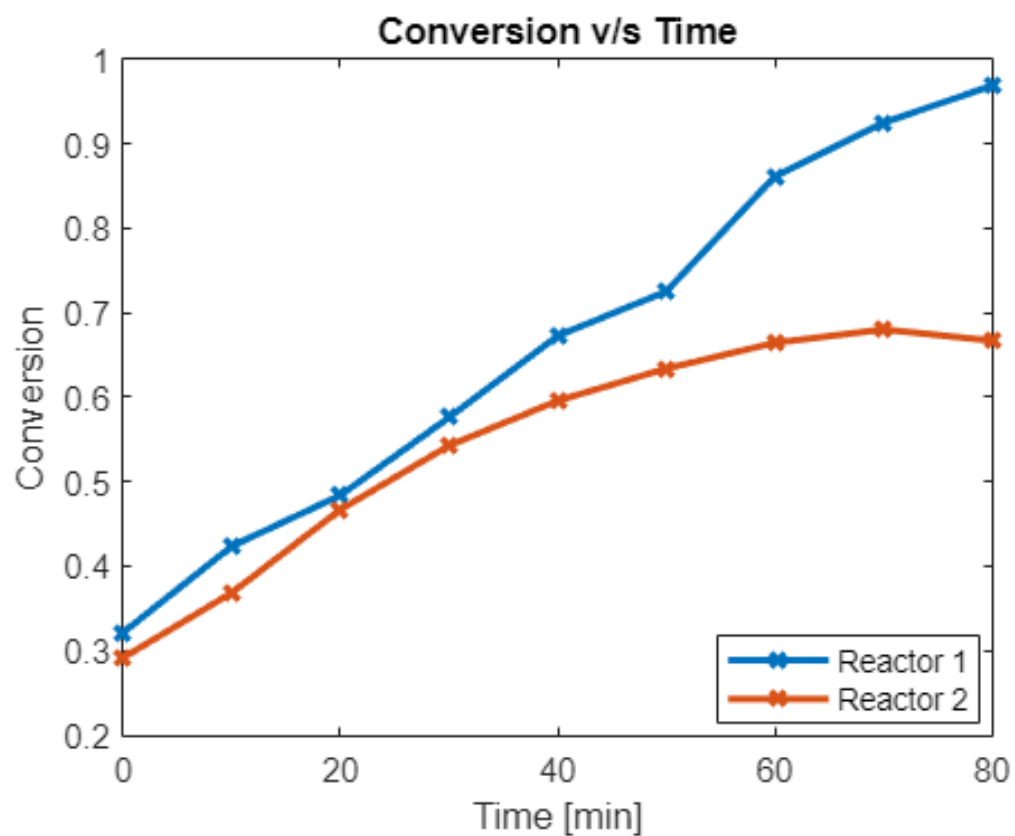
```
plot(t, T_r1, 'LineWidth', 2)
hold on
plot(t, T_r2, 'LineWidth', 2)
title('Reactor Temperatures [degC] v/s Time (min)')
ylabel('Reactor Temperature [degC]')
xlabel('Time [min]')
legend('Reactor 1', 'Reactor 2', 'Location','best')
hold off
```



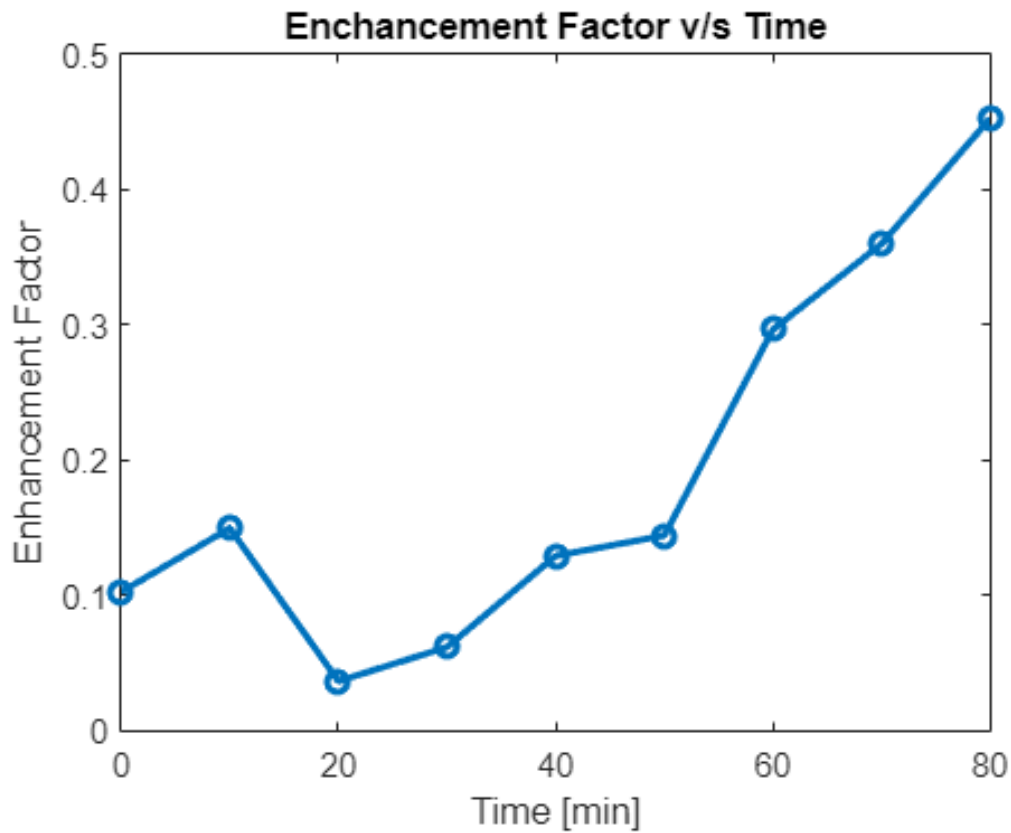
```
plot(t, cum_water_rem_r1, '-x','LineWidth',2)
xlabel('Time [min]')
ylabel('Cumulative Water Removed [mL]')
title('Cumulative water Removed in Reactor v/s Time')
```



```
plot(t,X1,'-x','LineWidth',2)
hold on
plot(t,X2,'-x','LineWidth',2)
xlabel('Time [min]')
ylabel('Conversion')
title('Conversion v/s Time')
legend('Reactor 1', 'Reactor 2', 'Location','best')
%ylim([0 1])
hold off
```



```
plot(t, E, '-o', 'LineWidth', 2)
hold on
xlabel('Time [min]')
ylabel('Enhancement Factor')
title('Enhancement Factor v/s Time')
hold off
```



```
% for Reactor 1
```

Writing to Excel

```
filename='MT_302.xlsx';
T=table(t',T_r1',water_lost',V_naoh_r1',vol_in_r1',X1');
T.Properties.VariableNames = {'Time','Temperature','Water Lost','NaOH required','Volume remaining'}
```

T = 9×6 table

...

|   | Time | Temperature | Water Lost | NaOH required | Volume remaining |
|---|------|-------------|------------|---------------|------------------|
| 1 | 0    | 100         | 0          | 9.1000        | 548              |
| 2 | 10   | 100.2000    | 16.5000    | 8             | 529.5000         |
| 3 | 20   | 104         | 15         | 7.4000        | 512.5000         |
| 4 | 30   | 113.5000    | 16         | 6.3000        | 494.5000         |
| 5 | 40   | 120.1000    | 11.5000    | 5             | 481              |
| 6 | 50   | 123.4000    | 9.5000     | 4.3000        | 469.5000         |
| 7 | 60   | 123.9000    | 5          | 2.2000        | 462.5000         |
| 8 | 70   | 124.2000    | 2          | 1.2000        | 458.5000         |

|   | Time | Temperature | Water Lost | NaOH required | Volume remaining |
|---|------|-------------|------------|---------------|------------------|
| 9 | 80   | 124.7000    | 1.3000     | 0.5000        | 455.2000         |

```
writetable(T,filename,'Sheet','reactor 1')
```

```
T1=table(t',T_r2',V_naoh_r2',X2');
```

```
T1.Properties.VariableNames = {'Time','Temperature','NaOH required','Conversion (X2)'}
```

T1 = 9×4 table

|   | Time | Temperature | NaOH required | Conversion (X2) |
|---|------|-------------|---------------|-----------------|
| 1 | 0    | 98.7000     | 9.5000        | 0.2917          |
| 2 | 10   | 97.4000     | 8.5000        | 0.3686          |
| 3 | 20   | 97          | 7.2000        | 0.4671          |
| 4 | 30   | 96.9000     | 6.2000        | 0.5428          |
| 5 | 40   | 96.4000     | 5.5000        | 0.5959          |
| 6 | 50   | 96.5000     | 5             | 0.6340          |
| 7 | 60   | 96.5000     | 4.6000        | 0.6645          |
| 8 | 70   | 96.6000     | 4.4000        | 0.6803          |
| 9 | 80   | 96.5000     | 4.6000        | 0.6670          |

```
writetable(T1,filename,'Sheet','reactor 2')
```

```
results = table(t',X1',X2',E');
```

```
results.Properties.VariableNames={'Time','Conversion (X1)', 'Conversion (X2)', 'Enhancement Factor'}
```

results = 9×4 table

|   | Time | Conversion (X1) | Conversion (X2) | Enhancement Factor |
|---|------|-----------------|-----------------|--------------------|
| 1 | 0    | 0.3215          | 0.2917          | 0.1022             |
| 2 | 10   | 0.4237          | 0.3686          | 0.1495             |
| 3 | 20   | 0.4840          | 0.4671          | 0.0362             |
| 4 | 30   | 0.5761          | 0.5428          | 0.0614             |
| 5 | 40   | 0.6728          | 0.5959          | 0.1290             |
| 6 | 50   | 0.7253          | 0.6340          | 0.1440             |
| 7 | 60   | 0.8616          | 0.6645          | 0.2965             |
| 8 | 70   | 0.9251          | 0.6803          | 0.3599             |
| 9 | 80   | 0.9690          | 0.6670          | 0.4527             |

```
writetable(results,filename,'sheet','Results')
```



