

```

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

```

```

vol_in_r1 = 1x9
    548.0000    529.5000    512.5000    494.5000    481.0000    469.5000    462.5000    458.5000 ...

```

```

n_acid_reacted_r1 = (vol_in_r1.*conc_acid_r1)/1000;
X1 = (n_ac-n_acid_reacted_r1)/(n_ac);

V_W_naoh = [0, 9, 7.1, 6.1, 5.1, 4.1, 4.4, 2.4, 1.5];
V_W = 5; % ml
acid_lost = ((1.*V_W_naoh)/V_W).*water_lost % in millimoles

```

```

acid_lost = 1x9
     0    29.7000    21.3000    19.5200    11.7300     7.7900     4.4000     0.9600 ...

```

```

total_acid_lost=sum(acid_lost)

```

```

total_acid_lost = 95.7900

```

```

%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
```

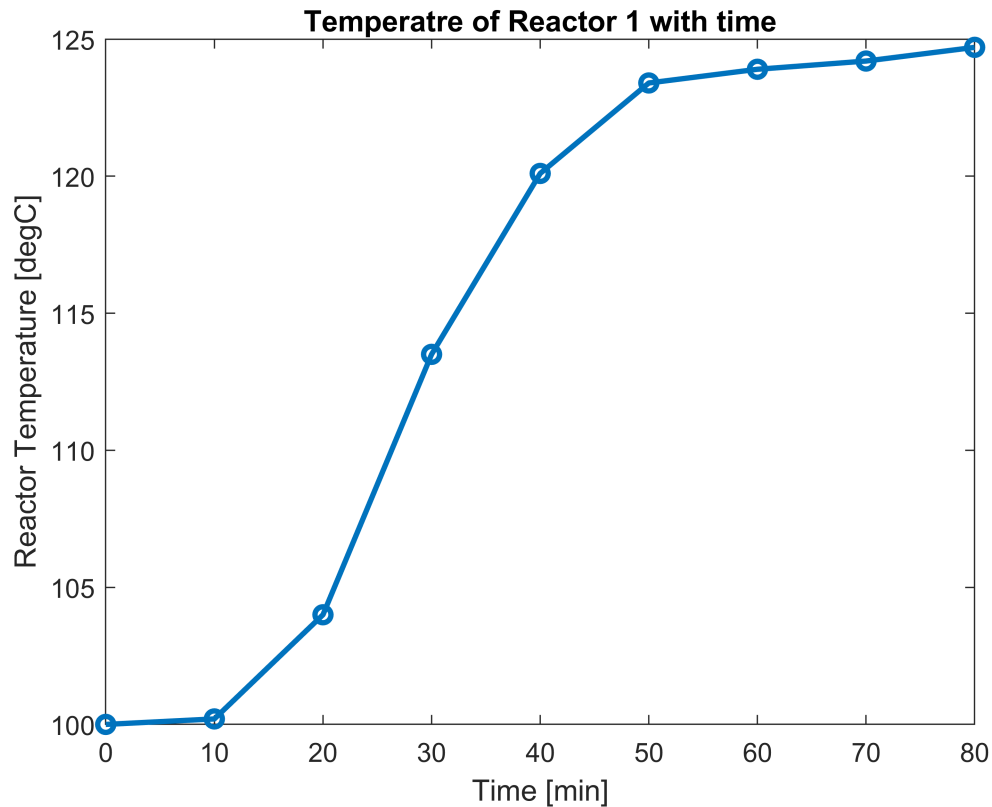
```
%Plots
```

```
plot(t, T_r1, '-o', 'LineWidth', 2)
```

```
title('Temperatre of Reactor 1 with time')
```

```
ylabel('Reactor Temperature [degC]')
```

```
xlabel('Time [min]')
```

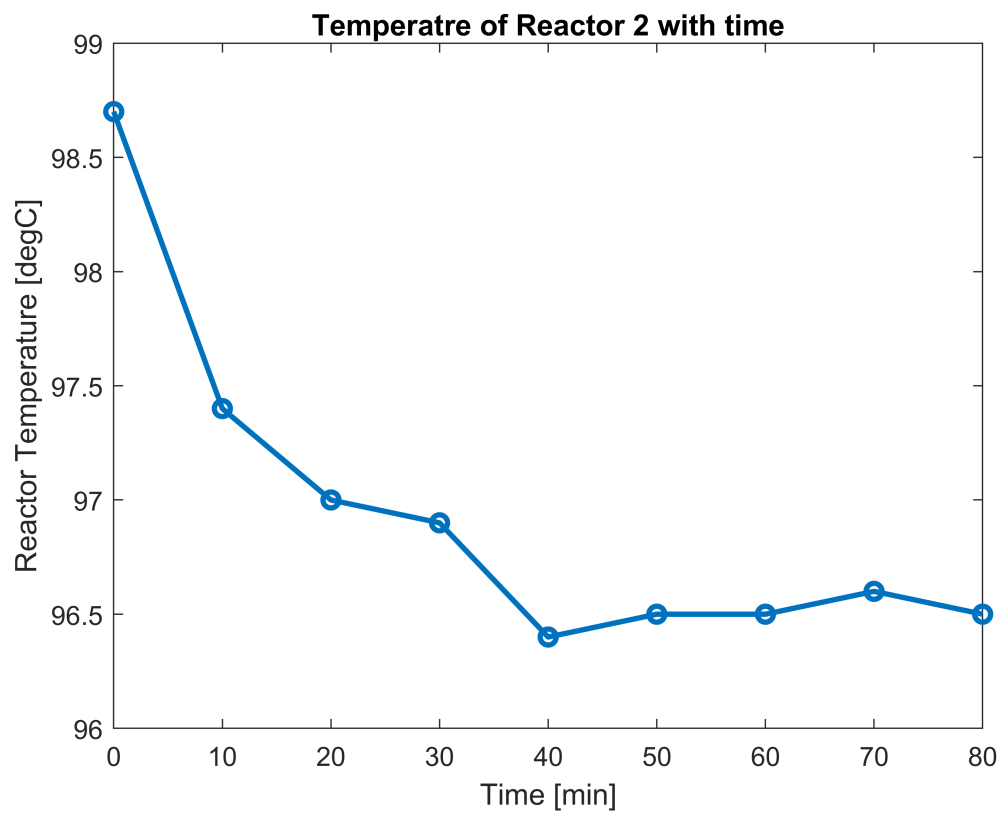


```
plot(t, T_r2, '-o', 'LineWidth', 2)
```

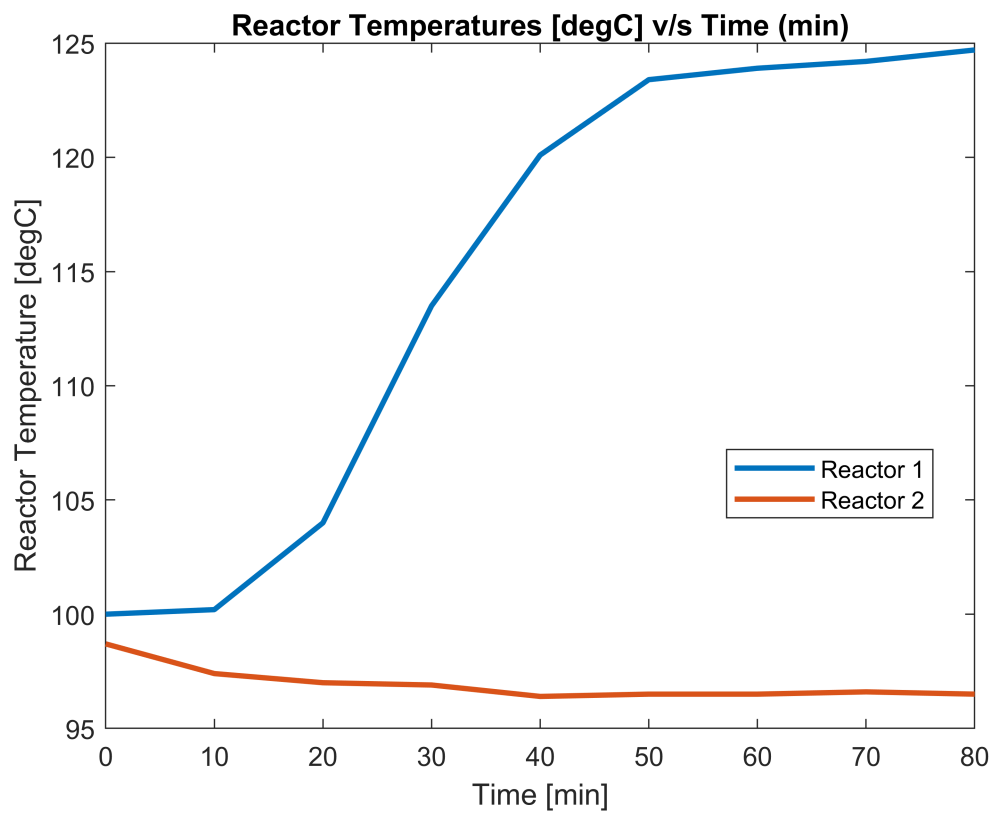
```
title('Temperatre of Reactor 2 with time')
```

```
ylabel('Reactor Temperature [degC]')
```

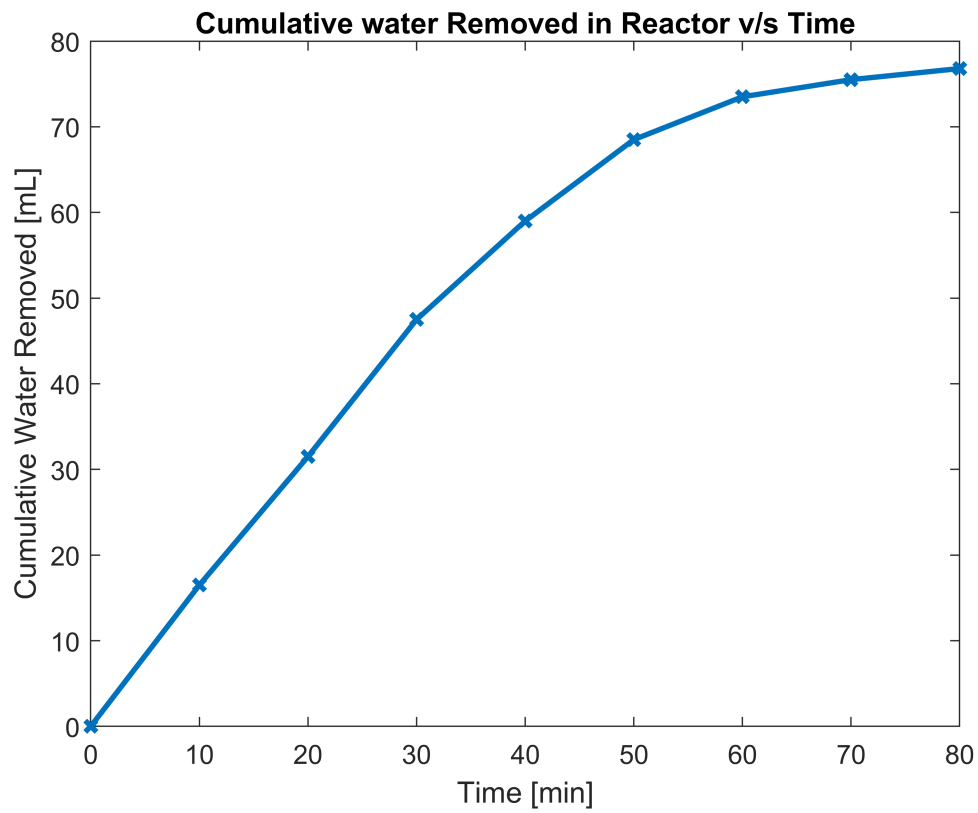
```
xlabel('Time [min]')
```



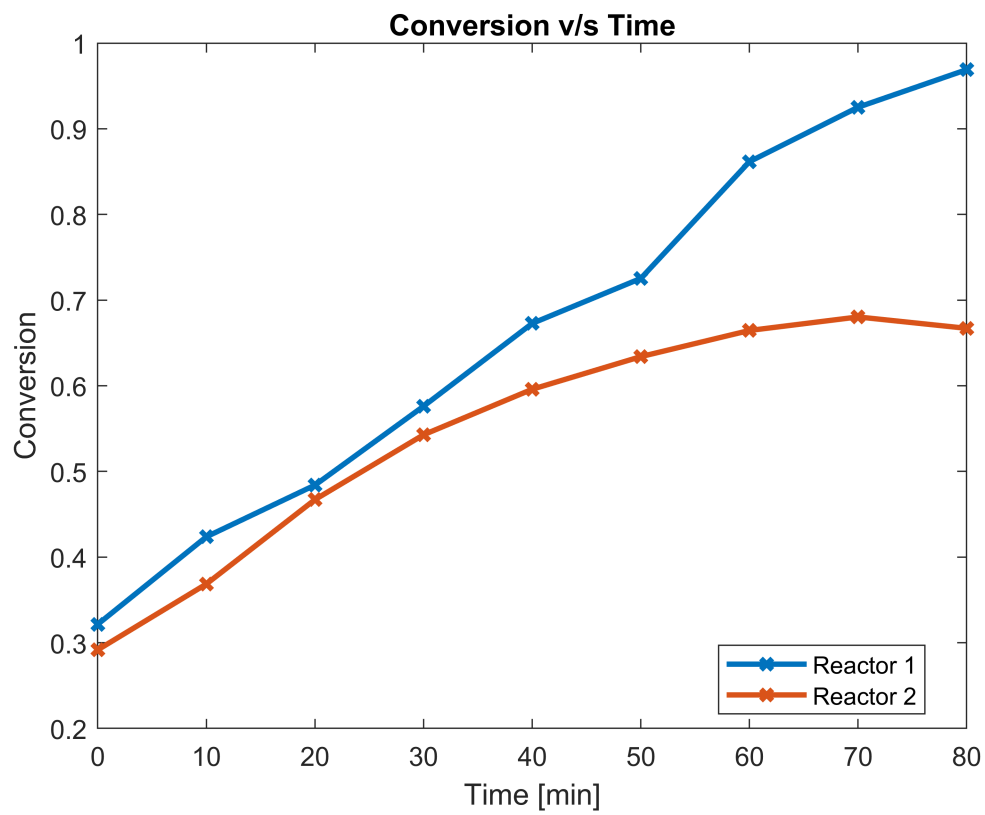
```
plot(t, T_r1, 'LineWidth', 2)
hold on
plot(t, T_r2, 'LineWidth', 2)
title('Reactor Temperatures [degC] v/s Time (min)')
ylabel('Reactor Temperature [degC]')
xlabel('Time [min]')
legend('Reactor 1', 'Reactor 2', 'Location','best')
hold off
```



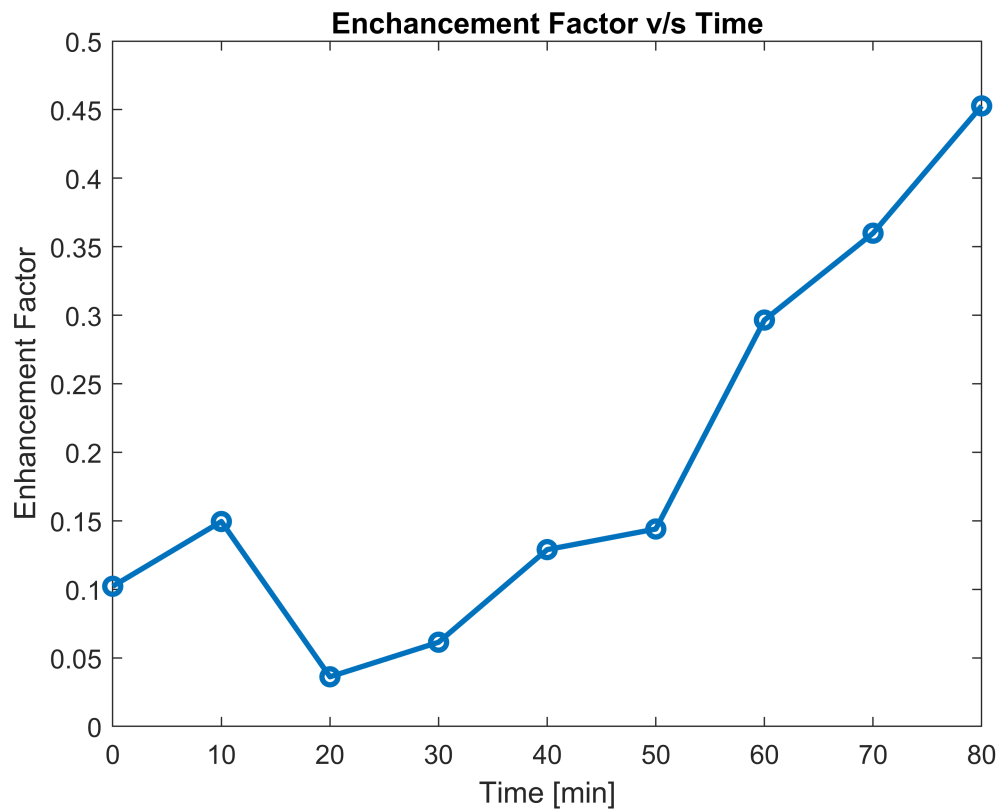
```
plot(t, cum_water_rem_r1, '-x','LineWidth',2)
xlabel('Time [min]')
ylabel('Cumulative Water Removed [mL]')
title('Cumulative water Removed in Reactor v/s Time')
```



```
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',acid_lost',V_naoh_r1',vol_in_r1',X1');
T.Properties.VariableNames = {'Time','Temperature','Water Lost','Acid Lost','NaOH required','Vol In','X1'};
```

T = 9×7 table

...

	Time	Temperature	Water Lost	Acid Lost	NaOH required
1	0	100	0	0	9.1000
2	10	100.2000	16.5000	29.7000	8
3	20	104	15	21.3000	7.4000
4	30	113.5000	16	19.5200	6.3000
5	40	120.1000	11.5000	11.7300	5
6	50	123.4000	9.5000	7.7900	4.3000
7	60	123.9000	5	4.4000	2.2000
8	70	124.2000	2	0.9600	1.2000

	Time	Temperature	Water Lost	Acid Lost	NaOH required
9	80	124.7000	1.3000	0.3900	0.5000

```
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')
```



