

analysis

May 13, 2023

1 Modules

```
[ ]: import pandas as pd
import matplotlib.pyplot as plt
import numpy as np
```

2 Data

```
[ ]: Tc = 273.65 # K
Th = 292.65 # K
T_catalysis = 292.65 # K
data_Tc = pd.read_csv("reaction-Tc.txt")
data_Th = pd.read_csv("reaction-Th.txt")
```

```
[ ]: data_Tc
```

```
[ ]: VKMnO4(L)  Vwater(L)  t(s)
0      0.0050      0.0000      0
1      0.0040      0.0010     317
2      0.0030      0.0020     615
3      0.0025      0.0025     811
4      0.0020      0.0030     968
5      0.0010      0.0040    1065
```

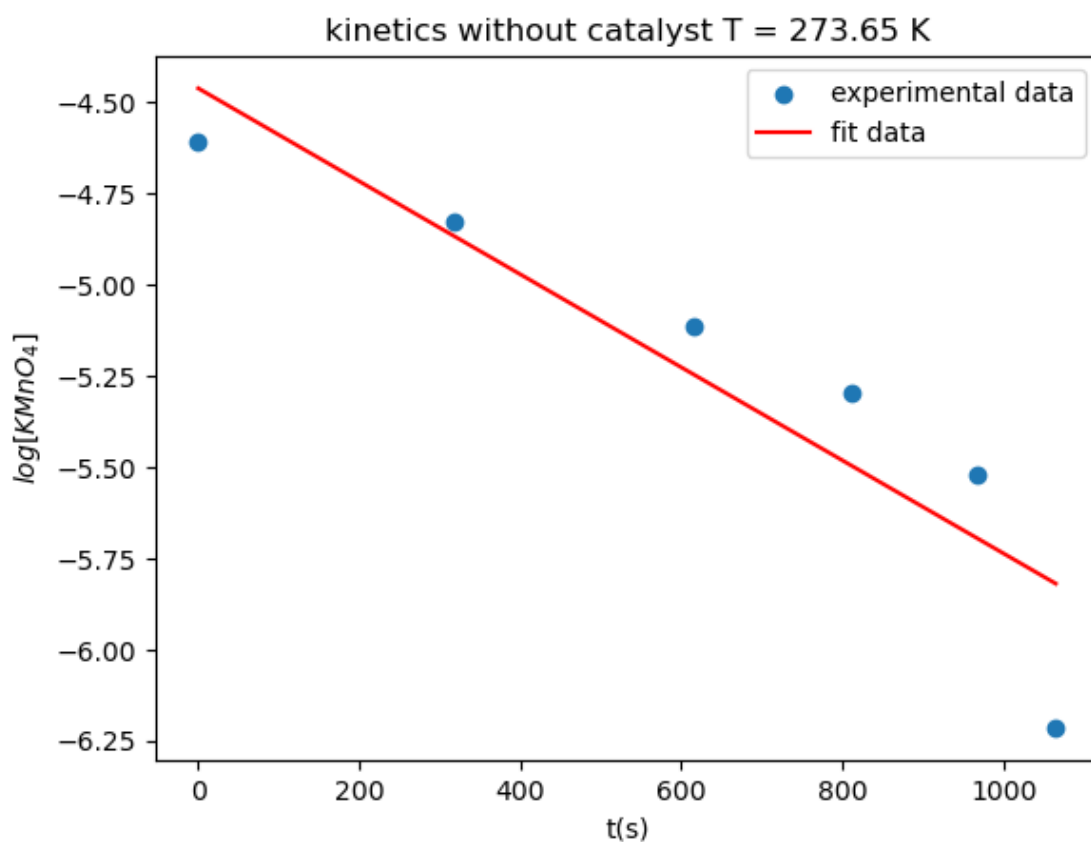
```
[ ]: data_Th
```

```
[ ]: VKMnO4(L)  Vwater(L)  t(s)
0      0.0050      0.0000      0
1      0.0040      0.0010     21
2      0.0030      0.0020     51
3      0.0025      0.0025     69
4      0.0020      0.0030     92
5      0.0010      0.0040    114
```

3 Rate constants

3.1 T_c

```
[ ]: concentration_Tc = (data_Tc["VKMnO4(L)"] * 0.01) / (data_Tc["VKMnO4(L)"] +  
    ↪ data_Tc["Vwater(L)"])  
  
fig, ax = plt.subplots()  
ax.scatter( data_Tc["t(s)"] , np.log( concentration_Tc ) , label = "experimental_  
    ↪ data" )  
ax.set_xlabel("t(s)")  
ax.set_ylabel("$\log[\text{KMnO}_4]$")  
ax.set_title("kinetics without catalyst T = "+str(Tc)+" K")  
  
coeff , cov = np.polyfit( data_Tc["t(s)"] , np.log( concentration_Tc ) ,  
    ↪ 1, cov=True)  
fit = np.poly1d(coeff)  
  
ax.plot( data_Tc["t(s)"] , fit( data_Tc["t(s)"] ) , color = "red" , label =  
    ↪ "fit data" )  
plt.legend()  
plt.show()
```



```
[ ]: concetration_Tc
```

```
[ ]: 0    0.010
      1    0.008
      2    0.006
      3    0.005
      4    0.004
      5    0.002
      dtype: float64
```

```
[ ]: k_c = round( -coeff[0] , 4 )
      deltak_c = round( np.sqrt( cov[0][0] ) , 4 )
      "The rate constant is (" + str( k_c )+ " +- "+str(deltak_c) + ") s^-1"
```

```
[ ]: 'The rate constant is (0.0013 +- 0.0003) s^-1'
```

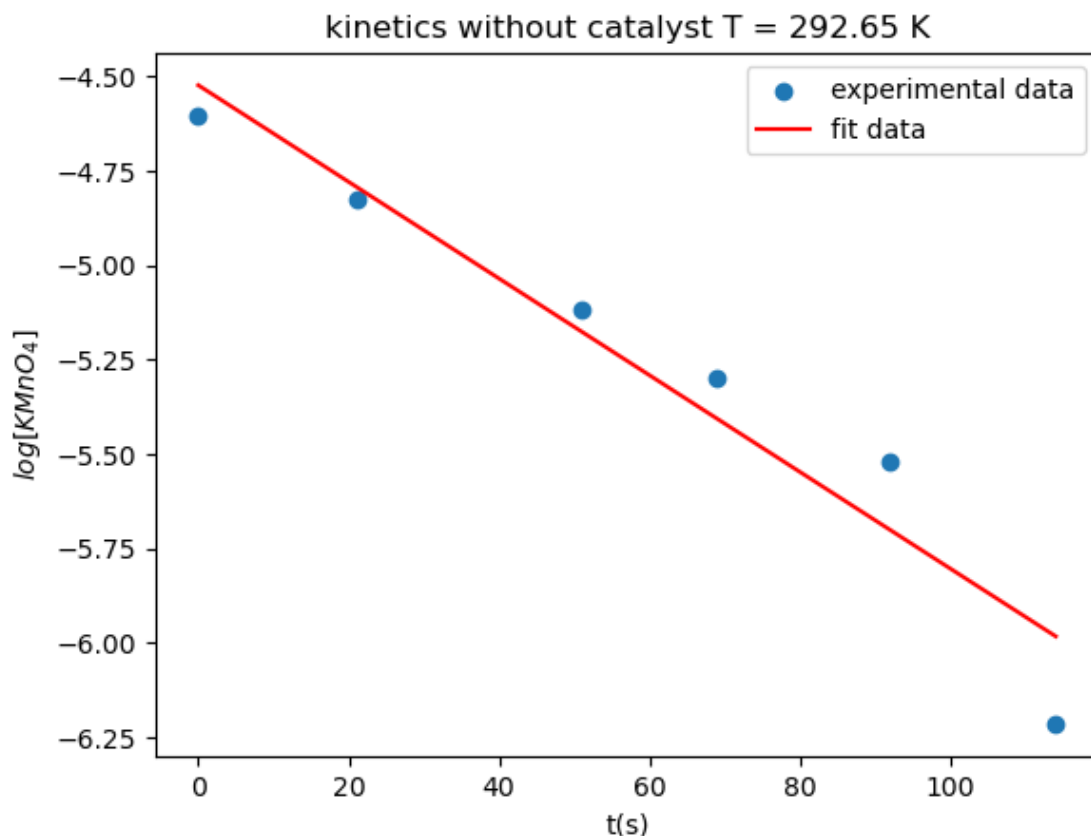
3.2 *Th*

```
[ ]: concetration_Th = (data_Th["VKMnO4(L)"] * 0.01)/ (data_Th["VKMnO4(L)"] +
      ↪data_Th["Vwater(L)"])

fig,ax = plt.subplots()
ax.scatter( data_Th["t(s)"] , np.log( concetration_Th ) , label = "experimental_
      ↪data" )
ax.set_xlabel("t(s)")
ax.set_ylabel("$log[KMnO_4]$")
ax.set_title("kinetics without catalyst T = "+str(Th)+" K")

coeff , cov = np.polyfit( data_Th["t(s)"] , np.log( concetration_Th ) ,
      ↪1,cov=True)
fit = np.poly1d(coeff)

ax.plot( data_Th["t(s)"] , fit( data_Th["t(s)"] ) , color = "red" , label =
      ↪"fit data" )
plt.legend()
plt.show()
```



```
[ ]: k_h = round( -coeff[0] , 3 )
      deltak_h = round( np.sqrt( cov[0][0] ) , 3 )
      "The rate constant is (" + str( k_h )+ " +- "+str(deltak_h) + ") s^-1"
```

```
[ ]: 'The rate constant is (0.013 +- 0.002) s^-1'
```

4 Energy activation

```
[ ]: R = 8.314*1e-3
      E = round( np.log( k_c / k_h ) * ( ( Tc*Th ) / ( Tc-Th ) ) * R )

      deltaE_k_c = ( deltak_c / k_c ) * ( ( Tc*Th ) / ( Tc-Th ) ) * R
      deltaE_k_h = ( deltak_h / k_h ) * ( ( Tc*Th ) / ( Tc-Th ) ) * R

      deltaE = round( np.sqrt( deltaE_k_h**2 + deltaE_k_c**2 ) )

      "The energy activation is ( " + str(E) + " +- " + str(deltaE) + " ) KJ /mol "
```

```
[ ]: 'The energy activation is ( 81 +- 10 ) KJ /mol '
```

5 Frequency factor

It can be shown that $A = \frac{k_c + k_h}{e^{-E/(R*T_c)} + e^{-E/(R*T_h)}}$

```
[ ]: A = round( ( ( k_c + k_h ) / ( np.exp( -E/(R*Tc) ) + np.exp( -E/(R*Th) ) ) ) * 1e-12 , 1)

"The frequency factor is " + str(A) + " e^12 s^-1"

[ ]: 'The frequency factor is 3.7 e^12 s^-1'
```

6 half life 20°C

```
[ ]: half_life = round( -np.log(1/2) / k_h )

"The half life of the reaction in 20°C is " + str(half_life) + " s"

[ ]: 'The half life of the reaction in 20°C is 53 s'
```

7 Note

If we have a initial concetration of A_0 and we need to arrive to concetration of B , the time used is

$$t = \frac{\ln A_0}{k} - \frac{\ln B}{k}$$

From the above we conclude that if the initial concentration is increased, there is a longer time to reach a fixed final concentration. Since it is not feasible to measure the concentration for different instants of time, we use a different method given by the following equation:

$$t_i = t^+ - t'_i$$

Where t_i is the time when te concetration is C_i , t'_i is time for complete the reaction when the concetration is C_i and t^+ is the time for complete the reaction when the concetration is $\max\{C_i\}_i$

Using the above we have concentration vs. time data for a reaction with initial concentration $\max\{C_i\}_i$