analysis2

August 7, 2023

1 Modules

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

2 Data

[ ]:
```python
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")
```

[ ]:
```python
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

[ ]:
```python
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

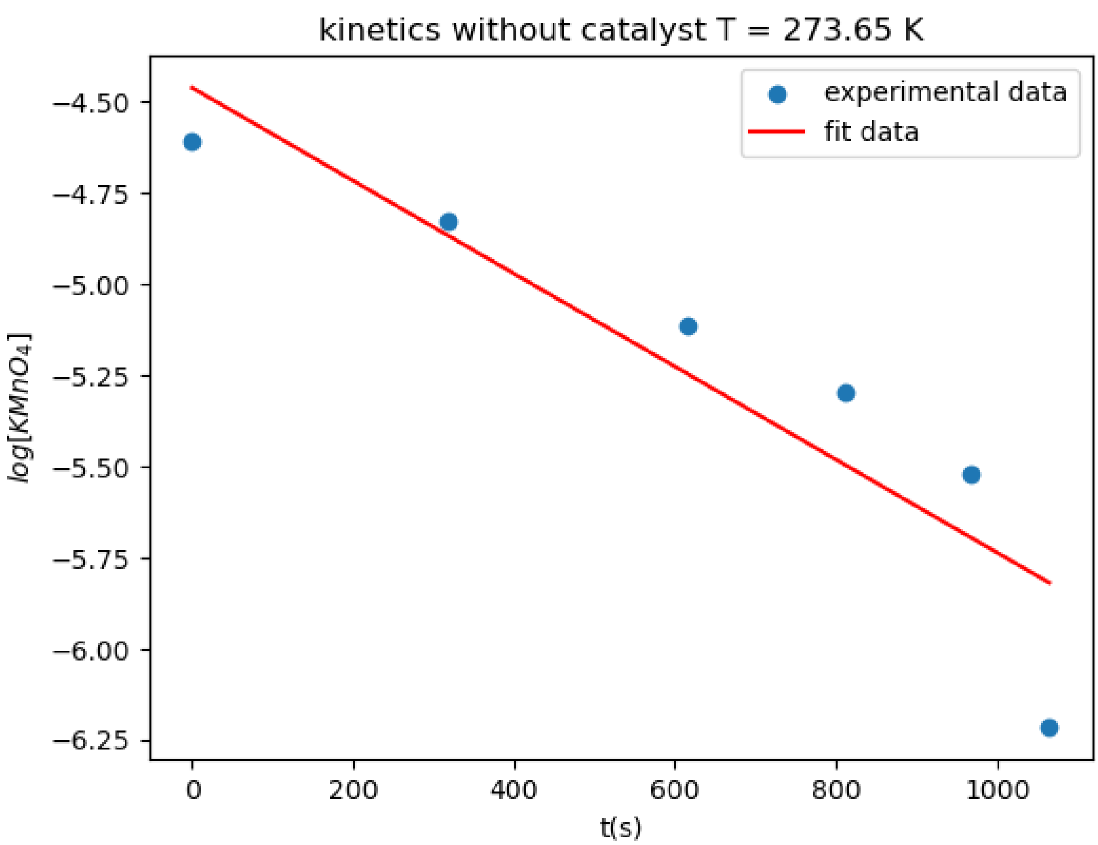
3.1 Tc

[ ]:
```
concetration_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( concetration_Tc ) , label = "experimental␣
↪data" )
ax.set_xlabel("t(s)")
ax.set_ylabel("$log[KMnO_4]$")
ax.set_title("kinetics without catalyst T = "+str(Tc)+" K")

coeff , cov = np.polyfit( data_Tc["t(s)"] , np.log( concetration_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'
```

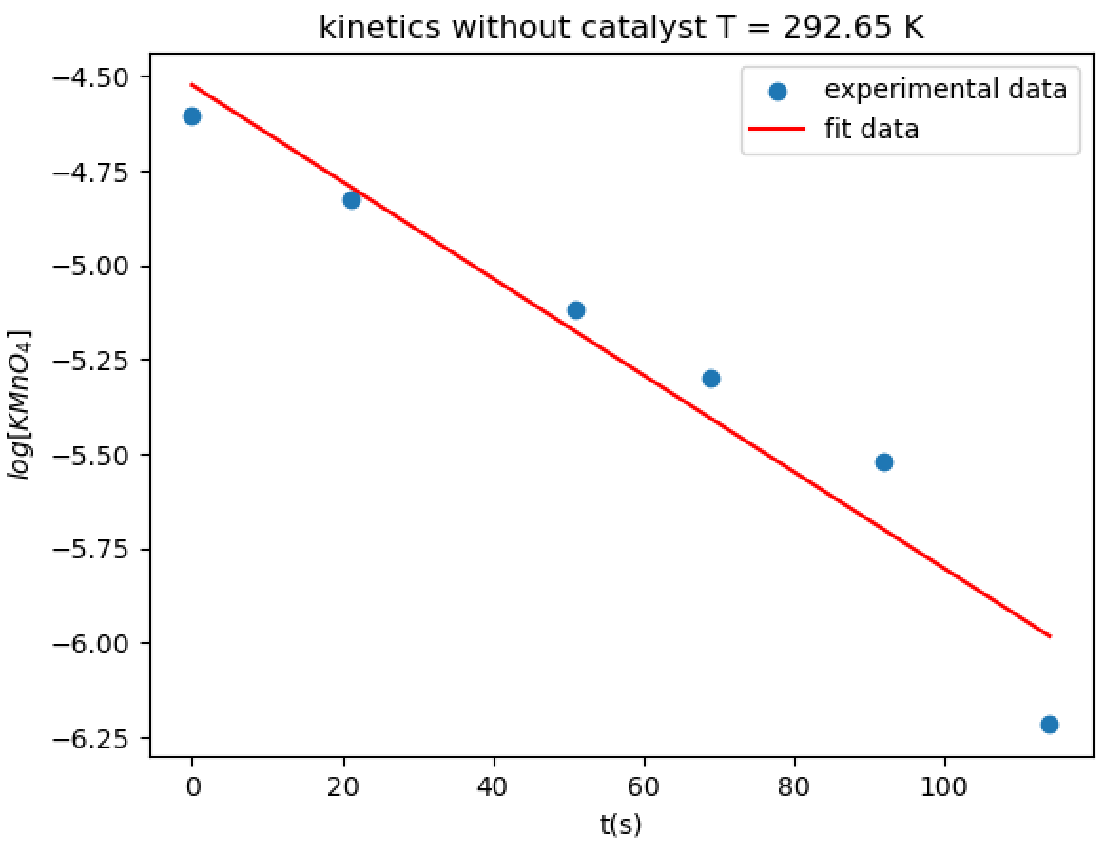
3.2 Th

[ ]:
```
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 Frecuency factor

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

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

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

[ ]: 'The frecuency 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 $t = \frac{lnA_0}{k} - \frac{lnB}{k}$

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 $max\{C_i\}_i$