465 Homework 4–Due 10/30/20@ 12:00pm (Noon) Jeremy Hook

In [162]:
```
import numpy as np
import matplotlib.pyplot as plt
from scipy.stats import linregress
import numpy as np                        # for scientific functions - mostly numerical
from matplotlib import pyplot as plt  # for plotting
from scipy.optimize import leastsq    # the function to carry out leastsquare optimization
```

PROBLEM # 1

1)You are living in a tropical paradise. Food is plentiful. The sun is shining. People no longer feel ashamed about their Nickelback CD collections. Humanity has evolved. You are now free to engineerwhatever you desire. Your next experimentis on determining the reaction order of a reaction for the synthesis of chemical X, which can be used to catalyze the formation of artificial chocolate(cacao). You take a container labeled “reagents”off the shelf and pour it into an isothermal, isobaric batch reactor and monitor the concentration over time. You suspect the reaction has the chemical equation A --> X and is irreversible.

time(min)012345678910

CA(mol/L)1.3370.8130.5710.4380.3630.3040.2670.2290.2070.1910.173

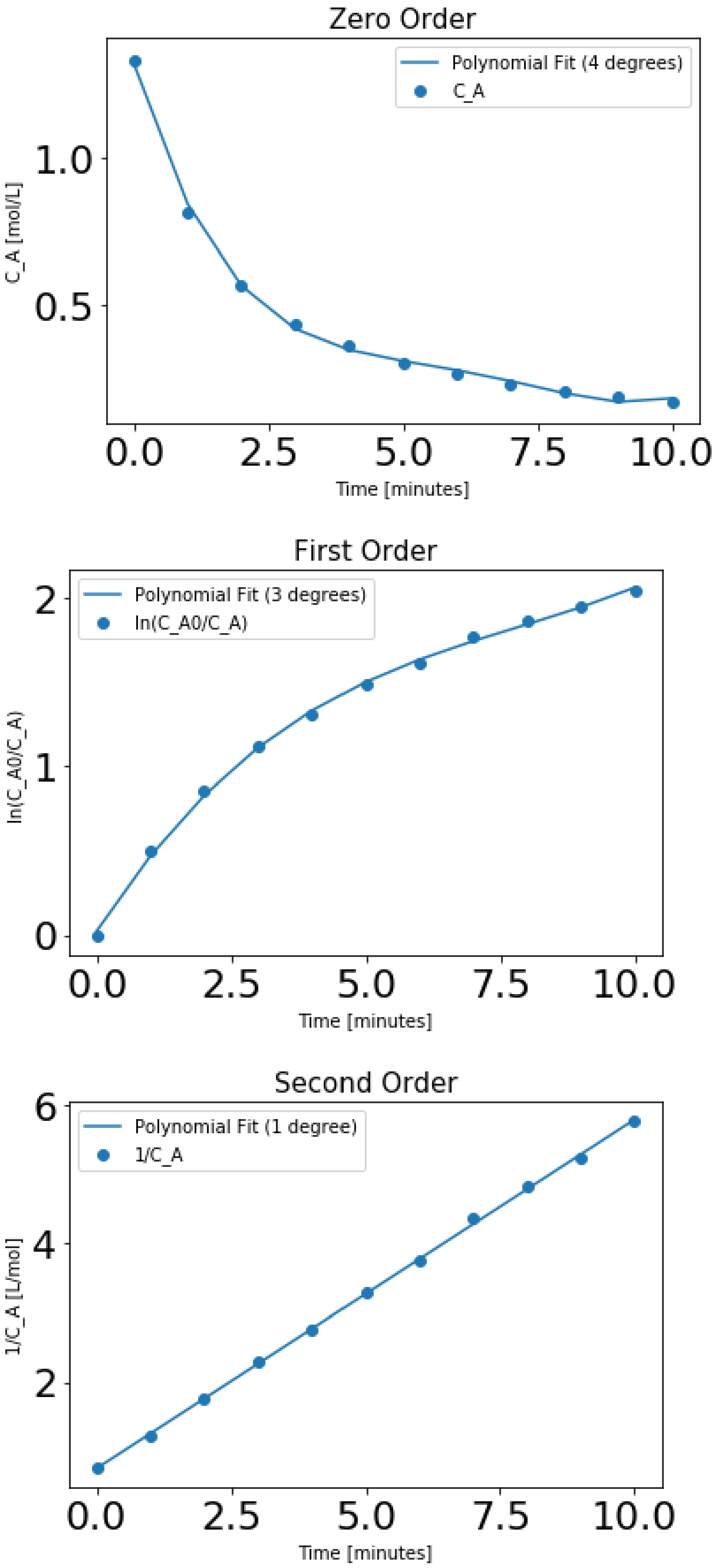
In [163]:
```
time = np.array([0,1,2,3,4,5,6,7,8,9,10]) #Minutes
C_A = np.array([1.337,0.813,0.571,0.438,0.363,0.304,0.267,0.229,0.207,0.191,0.173]) #mol/L
```

a.Using the Integral Method, find the order of the reaction. Create a plotin Python with the kinetic data and your fitted line with the appropriate axes for the order of the reaction. Be sure to label the axes (with units, if applicable) and give it a legend.

In [164]:

```
fig = plt.figure()
#Guess 1: zero order

plt.scatter(time, C_A, label ="C_A")
m0, b0, c0, d0, e0 = np.polyfit(time, C_A, 4) #Best-fitted line
plt.plot(time, m0*time**4+b0*time**3+c0*time**2+d0*time+e0 ,label ="Polynomial Fit (4 degrees)")
plt.title("Zero Order",size = '15')
plt.xlabel("Time [minutes]",size = '10')
plt.ylabel("C_A [mol/L]",size = '10')

plt.legend(prop={"size":10})

#Guess 2: first order
plt.figure()
ln = np.log(C_A[0]/C_A)
plt.scatter(time, ln, label ="ln(C_A0/C_A)")
m1, b1, c1, d1 = np.polyfit(time, ln, 3) #Best-fitted line
plt.plot(time, m1*time**3+b1*time**2+c1*time+d1, label ="Polynomial Fit (3 degrees)")
plt.title("First Order",size = '15')
plt.xlabel("Time [minutes]",size = '10')
plt.ylabel("ln(C_A0/C_A)",size = '10')
plt.legend(prop={"size":10})

#Guess 3: second order
plt.figure()
inv = (1/C_A)
plt.scatter(time, inv, label ="1/C_A")
m2, b2 = np.polyfit(time, inv, 1) #Best-fitted line
plt.plot(time, m2*time+b2, label ="Polynomial Fit (1 degree)")
plt.title("Second Order",size = '15')
plt.xlabel("Time [minutes]",size = '10')
plt.ylabel("1/C_A [L/mol]",size = '10')
plt.legend(prop={"size":10})
```

```
Out[164]: <matplotlib.legend.Legend at 0x19dc6244a88>
```


Zero Order
Polynomial Fit (4 degrees)
C_A
C_A [mol/L]
1.0
0.5
0.0
2.5
5.0
7.5
10.0
Time [minutes]
First Order
Polynomial Fit (3 degrees)
ln(C_A0/C_A)
ln(C_A0/C_A)
2
1
0
0.0
2.5
5.0
7.5
10.0
Time [minutes]
Second Order
Polynomial Fit (1 degree)
1/C_A
1/C_A [L/mol]
6
4
2
0.0
2.5
5.0
7.5
10.0
Time [minutes]

Due to the linear fit of the data to our "Second Order" plot we can see that the order of the reaction is 2

b.From your fit in part a, what is the reaction rate constant for this process?

In [165]:

```
#We can see from part a that this is a second order process, because it has a
 linear fit which is 1/C_A = 1/C_A0 + kt
k = m2 # The slope of this linear fit will be out k value
print('Reaction rate constant (k)= {:.5f} [L /(mol)(min)]'.format(k))
```

```
Reaction rate constant (k)= 0.50528 [L /(mol)(min)]
```

c.After reading the container of “reagents”more carefully,you realize that the chemical equation for the reaction was actually 2A + B --> X all alongand the reaction follows an elementary rate law. It also says that the reaction rate constant is 0.02 L2mol-2min-1. Given this new information, what was the concentration of B if it was held constant when the tabulated data was gathered.

In [166]:

```
#Reaction: 2A + B --> X, k = .02 [L^2/(mol^2*min)]
#The reaction follows an  elementary  rate  law = -r_A = -dC_A/dt = k*C_A^2*C_
B
k = 0.02  # [L^2/(mol^2*min)]

C_B = ((-1/C_A[10])-(-1/C_A[0]))/(-k*(time[10]-time[0])) #To find concentratio
n of C_B rearrange equation above and solve the differential to to solve for C
_B
print('If C_B was held constant C_B = {:.5f} [mol/L]'.format(C_B))
```

```
If C_B was held constant C_B = 25.16202 [mol/L]
```

PROBLEM # 2

2)Kinetic rate data (which can be found on Canvas) is given for a chemical reaction A --> B, but the order of the reaction is not known. The reaction occurred in an isothermal, isobaric batch reactor. The units of the concentration data are in mol/L and time is in minutes.

In [172]:

```
cA = np.array([9.871507338462981451e+00,7.043182012988722818e+00,5.74692461466
7721087e+00,4.971537585096347023e+00,4.457849128909017189e+00,4.06496028633292
1946e+00,3.772592721342783229e+00,3.514160649290875238e+00,3.31984500814574801
1e+00,3.160456588877444517e+00,3.009833424250920597e+00,2.879221218135621374e+
00,2.772167910991736317e+00,2.663273581787786171e+00,2.578182658197410326e+00,
2.493854311651262368e+00,2.419711253693596298e+00,2.354660875889686533e+00,2.2
91649331325676275e+00,2.232809013822000477e+00,2.178239995714944754e+00,2.1310
97725638296136e+00]) #mol/L
```

In [173]:

```
t = np.array([0.000000000000000000e+00,5.000000000000000000e-01,1.0000000000000
00000e+00,1.500000000000000000e+00,2.000000000000000000e+00,2.5000000000000000
00e+00,3.000000000000000000e+00,3.500000000000000000e+00,4.000000000000000000e
+00,4.500000000000000000e+00,5.000000000000000000e+00,5.500000000000000000e+00
,6.000000000000000000e+00,6.500000000000000000e+00,7.000000000000000000e+00,7.
500000000000000000e+00,8.000000000000000000e+00,8.500000000000000000e+00,9.000
000000000000000e+00,9.500000000000000000e+00,1.000000000000000000e+01,1.050000
000000000000e+01]) #Minutes
```

a.Use the Differential Method to determine the order of the reaction given the kinetic rate data. You may round to the nearest integer. It would be best to perform these calculations in Python (np.diff()is very helpful here).

In [174]:

```
#Differential Method ln(-dCA/dt) = ln(kA) + alpha * ln(CA)
#plot ln(-dCA/dt) vs ln(CA)

ln_CA = np.log(cA)
diff_CA = np.diff(cA)
diff_time = np.diff(t)

delta_time = diff_time[0]
natlog_derivative = np.double(np.arange(0,22))
natlog_derivative[0] = np.double(np.log(-((-3)*cA[0] +4*cA[1] - cA[2])/(2*delt
a_time)))
natlog_derivative[21] = np.double(np.log(-((3)*cA[21] -4*cA[20] + cA[19])/(2*d
elta_time)))

for i in range(1,21):
    natlog_derivative[i] = np.double(np.log(-(cA[i+1]-cA[i-1])))

#From the data we have created we could fit a polynomial line to the data, and
whatever the slope of this polynomial line is will be our alpha value which wi
ll be the Order of the reaction
m, b = np.polyfit(ln_CA, natlog_derivative, 1) #Polynomial fit line
alpha = m #The slope of our polynomial fit line

print('The Order of Reaction (alpha) = {:.0f}'.format(alpha))
```

```
The Order of Reaction (alpha) = 3
```

b.Calculate the rate constant of the reaction as well with the proper units.

In [175]:

```
#Equation 7-11 from FOLDGER BOOK
#because k is a constant rate change we only need to choose a point from the c
oncentration A and then find the derivative

k = np.exp((m*ln_CA[10]+b)/(alpha*ln_CA[10]))
print('Rate constant (k) =  {:.5f} [L^2/(mol^2)(min)]'.format(k))
```

```
Rate constant (k) =  0.67378 [L^2/(mol^2)(min)]
```

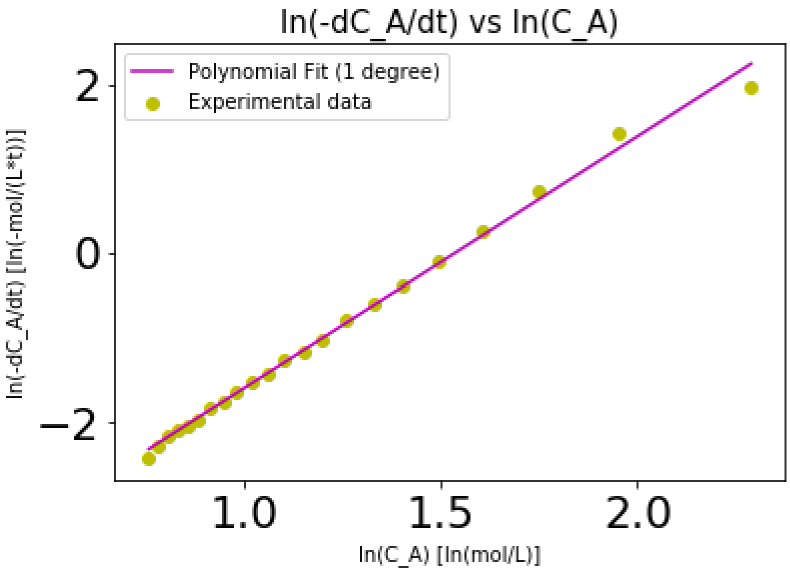
c.Include the plot of your fitted line and of the provided data with appropriately labeled axes.

In [176]:

```
#Plot Differential Method Using the information that we got in part A of this problem

plt.scatter(ln_CA, natlog_derivative, label ='Experimental data', color = 'y')
plt.plot(ln_CA, m*ln_CA+b,color = 'm', label ="Polynomial Fit (1 degree)")
plt.title("ln(-dC_A/dt) vs ln(C_A)",size = 15)
plt.xlabel("ln(C_A) [ln(mol/L)]",size = 10)
plt.ylabel("ln(-dC_A/dt) [ln(-mol/(L*t))]",size = 10)
plt.legend(prop={"size":10})
```

Out[176]:

```
<matplotlib.legend.Legend at 0x19dc6303688>
```



In [ ]:

In [ ]: