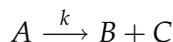


CHEN 1703 - HOMEWORK 9

Submit your solutions via the course web site. Be sure to include your name and UNID in your m-file.
Submit each solution separately. Also be sure to document your solutions well.

Problem 1 (20 pts)

In homework 5, we considered a chemical reaction where species A decomposes to form B and C ,



As you will learn in your kinetics class, there are a few possible ways that this reaction may proceed. From these, we obtain the following equations for the concentration of A , c_A as a function of time:

$$c_A = c_A^0 \exp(-kt) \quad \text{First order reaction} \quad (1)$$

$$c_A = \frac{c_A^0}{1 + kt c_A^0} \quad \text{Second order reaction} \quad (2)$$

Using the data shown in Table 1,

1. (10 pts) Use regression to determine k and c_A^0 for both a first order and a second order reaction.
2. (5 pts) Calculate the R^2 value for the data for the first order and second order reactions. Implement this as a function and save it in a file named `r_square.m`. Call this function from your main matlab file to calculate the R^2 values.
3. (5 pts) Plot the data, along with the predicted values for $c_A(t)$ using equations (1) and (2) with the regressed values for k and c_A^0 that you determined in part 1.

t (s)	0	0.43	0.86	1.29	1.71	2.14	2.57	3.00
c_A ($\frac{\text{mol}}{\text{cm}^3}$)	0.96	0.64	0.40	0.27	0.18	0.12	0.07	0.049

Table 1: The concentration of species A as a function of time.

Submit a report for this problem. Describe the approach you took to determine k and c_A^0 in part 1, report the R^2 values, and include your plots from part 3 in your report. Also submit your Matlab script.

Problem 2 (5 pts)

Revisit Homework 4, problem 2. Create a function to calculate ρ as a function of T using the ideal gas law. The function should take the following arguments:

- Molecular weight of the compound (in g/mol).
- A vector containing the temperatures (in Kelvin).

- The pressure (Pa).

Create a driver program that calls this function and generates the plot as described in Homework 4 problem 2. Submit your driver file and the function described above.

Problem 3 (5 pts)

Repeat homework 7, problem 2 and eliminate all `input` commands from that problem. Replace these with function arguments. Additionally, allow the user to specify the name of the output file as a function argument. Submit this function as your solution to this problem.