Reaction Order Determination Using Time and Concentration Data

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Assignment-01

1. Introduction

Understanding the kinetics of a chemical reaction is crucial for determining the reaction mechanism, optimizing conditions, and scaling up processes. Reaction order plays a fundamental role in describing how the concentration of reactants influences the rate of reaction. This project aims to identify the reaction order nnn by fitting different kinetic models to experimental data consisting of concentration and time values.

In this analysis, data from a reaction's progression is used to evaluate the fit for zero-order, first-order, second-order, and nth-order reaction models. The primary objective is to determine the reaction order that best describes the relationship between concentration and time.

2. Data and Methodology

The reaction data consists of concentration C (in mol/L) and time t (in seconds) as given:

Concentration(mol/l)	Time(sec)
10	0
8	20
6	40
5	60
3	120
2	180
1	300

Table 1: Experimentally obtained data for Concentration VS Time

The following steps were performed to analyze the reaction order:

For a zero-order reaction, the concentration (C) decreases linearly with time, verified by plotting C versus time (t). In a first-order reaction, the natural logarithm of concentration (ln(C)) decreases linearly with time, confirmed by fitting a linear regression to ln(C) versus t. In second-order kinetics, the reciprocal of concentration (1/C) increases linearly with time, tested by fitting a linear model to 1/C versus t. For nth-order reactions, a linear relationship is established between C^(1-n) and time, and various values of n are iterated to find the best fit based on the R^2 value.

3. Results and Discussion

The analysis resulted in the following R^2 values for different reaction order:

Order of Reaction(n)	R^2
Zero-order reaction	0.8081
First-order reaction	0.9790
Second-order reaction	0.9692

Table 2: Order of reaction and corresponding R^2 is shown

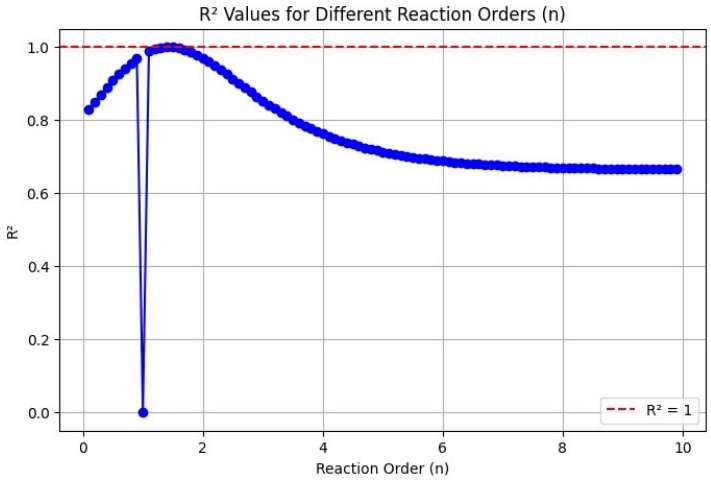

Figure 1 :R^2 for different reaction order

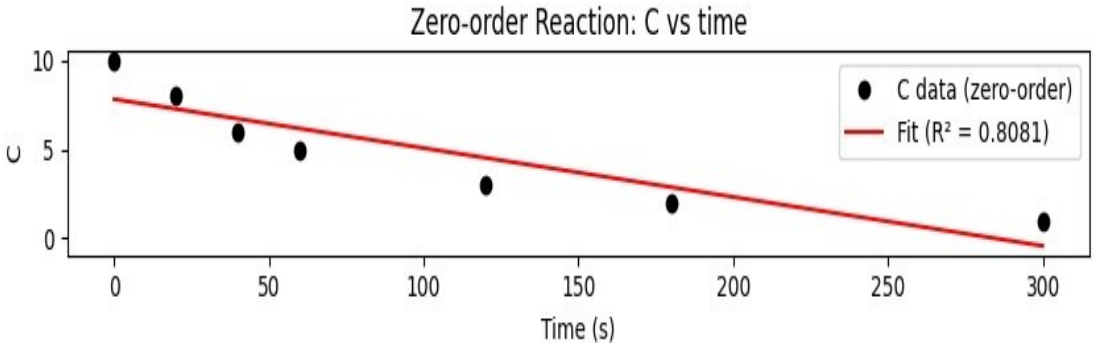

Figure 2 : Plot of concentration (C) versus time (t) for zero-order reaction showing linear decrease in C over time.

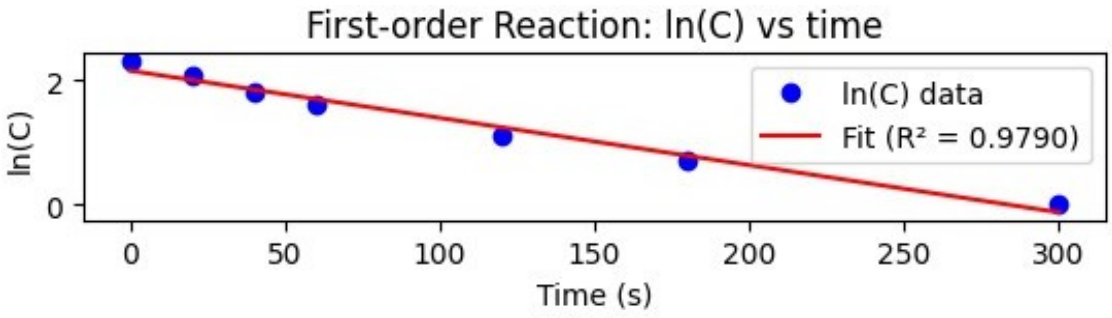

Figure 3: Plot of natural logarithm of concentration [ln(C)] versus time (t) for first-order reaction showing a linear trend.

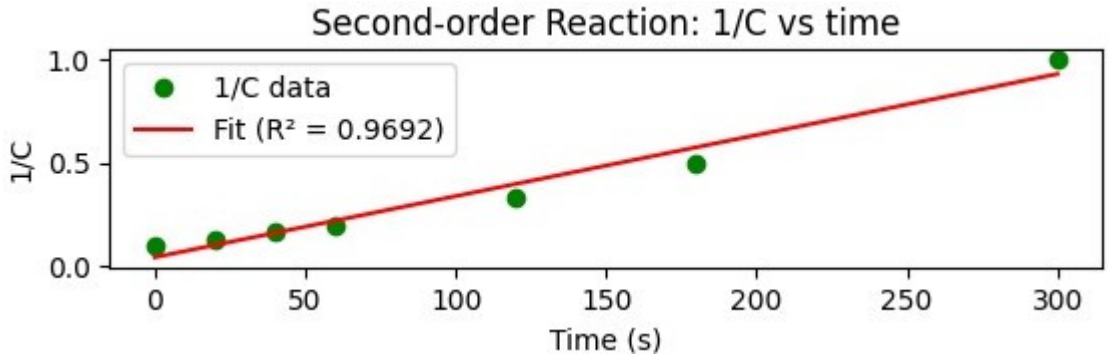

Figure 4: Plot of reciprocal of concentration (1/C) versus time (t) for second-order reaction showing linear increase in 1/C over time.

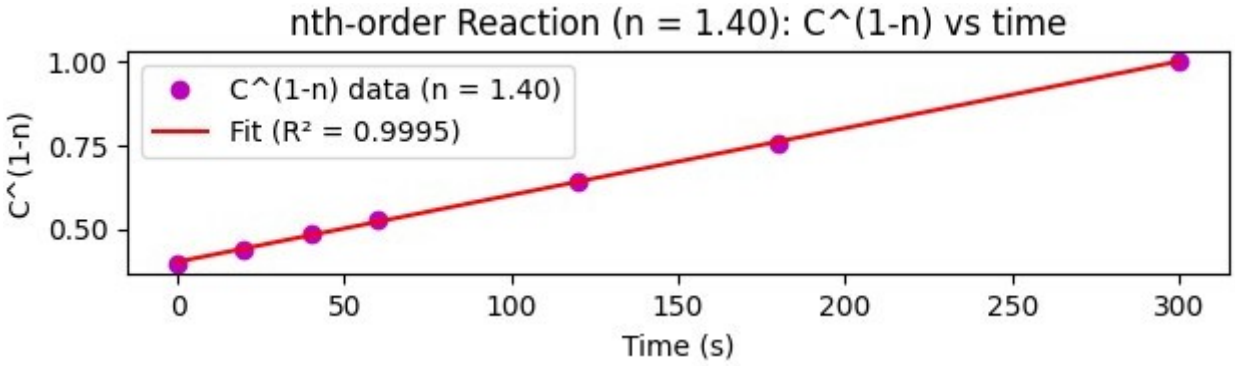

Figure 5: Plot of C^(1-n) versus time (t) for nth-order reaction, showing linear fit for various values of reaction order (n).

Rate Law Expression:

$$-r_A = \frac{-dC_A}{dt} = KC_A^{1.4} \quad [1]$$

$$C_A^{-0.4} - C_{A0}^{-0.4} = 0.4Kt \quad [2]$$

Rate Constant:

$$C_{A0} = 10\,mol/l\,, C_A = 8\,mol/l\,, t = 20\,sec\,, K = ?$$

Put the given data in equation [2]

$$K = 0.0046\left(\frac{mol}{l}\right)^{-0.4} s^{-1}$$

4. Conclusions

Through this assignment, the reaction order was systematically analyzed using different kinetic models. The results showed that the reaction is best described by an order n = 1.4 , indicating fractional-order kinetics. This finding could be indicative of complex reaction mechanisms or interactions among multiple species.

The zero-order model also provided a good fit, which could point toward reaction conditions where the rate becomes independent of concentration. Future work could involve analyzing more time points or using more complex models to further understand the reaction's behavior.

4. Additional Information

Git-Hub: https://github.com/karan-1310/Chemical-Reaction-Engineering

OR

Google Colab : https://colab.research.google.com/drive/10I4uSP9xirS-8AVazTTJpPl3n7xc_RRB?usp=sharing