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APPLICATION OF HIGHER MATHEMATICS TO CHEMISTRY: MODELING REACTION RATE USING DIFFERENTIAL EQUATIONS

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Abstract:
The article examines the application of higher mathematics to practical, in particular chemical processes, how to model the rate of a chemical reaction using differential equations, and reveals their meaning.

Keywords: Chemistry, chemical processes, chemical reaction rate, differential equations, modeling, integral, logarithm.

Introduction

The main goal of higher mathematics is to describe and analyze complex phenomena occurring in nature using mathematical models. Mathematical methods play an important role in chemistry in particular. Mathematical tools, in particular differential equations, are widely used to deeply understand the behavior of chemical processes. In this article, we will consider how to model the rate of a chemical reaction using differential equations.

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1. Reaction rate and its mathematical expression. In chemistry, the rate of a reaction is how the concentrations of the reactants change over time. For example, a simple reaction: A→B

The rate expression of the reaction:

$$\vartheta = -\frac{d(A)}{dt}$$

Here (A) is the concentration of the substance, t is time, and V is velocity.

In general, the reaction rate is as follows:

$$\vartheta = k(A)^n$$

Here:

k- rate constant;

n- reaction order.

2. Higher mathematics phenomenon: Differential equation. The differential equations branch of mathematics is used to express the dependence of variables on time. We write the differential equation for the reaction rate as:

$$\frac{d(A)}{dt} = -k(A)^n$$

This is a first-order ordinary differential equation. It describes how the amount of matter decreases over time.

3. Solution depending on the order of reaction

Level 1 reaction:

$$\frac{d(A)}{dt} = -k(A)^n$$

Integrating, we get:

ln(A) = −kt + ln(A0)

Level 0 reaction:

(A) = −kt + (A0)

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4. Chemical equilibrium and logarithmic equations.

Another important phenomenon in higher mathematics is logarithms. For example, the pH value, which is determined based on the concentration of hydrogen ions in water, is expressed as:

$$pH = -\log(H^+)$$

Also, the equilibrium constant (KC) and the acidity coefficient (pKa) are expressed in logarithmic form.

Differential equations are an important tool in mathematical modeling of chemical reaction rates. They are used to determine the time-dependent change in the concentration of a substance and analyze the dynamics of the reaction. This method is widely used in analyzing experimental results, optimizing reactions, and making scientific predictions.

The aboveLet's express each of the given information on modeling the rate of a chemical reaction using differential equations in the form of a chemical example.

1. Reaction rate and its mathematical expression. Combustion reaction with fuel and oxygen:

Let's assume that methane (CH_4) and oxygen (O_2) are reacting:

CH4+2O2→CO2+H2O

For this reaction to occur, the gases interact with each other at a certain rate. The rate of reaction is the change in the amount of products or reactants per unit of time.

How to measure the rate of a reaction in chemistry?

Let's observe the formation of carbon dioxide (CO_2) during the reaction. If we have an initial amount of CO_2 of 0 and after t seconds its amount is 0.1 moles, the reaction rate is:

$$\vartheta = \frac{\Delta[CO_2]}{\Delta t} = \frac{0.1\ \text{mol}}{t}$$

Mathematical expression: If [A] is the concentration of the reactant and the reaction is first order, then the reaction rate is written as:

$$\vartheta = k[A]$$

Here:

ϑ— reaction rate,
k— reaction rate constant,
[A] is the concentration of the reactant.

Conclusion:
To mathematically express the rate of chemical reactions, formulas that correspond to the order of the reaction are usually used. These formulas are related to the reaction time and help us understand how the reaction proceeds.

2. Higher mathematics phenomenon: Differential equation. The change in concentration with time in a first-order reaction:
Task: In reaction A, the initial concentration [A]0=2 mol/L. The reaction constant k=0.1 min-1. Find how the concentration of reactant A changes with time.
Differential equation:

$$\frac{d(A)}{dt} = -kA$$

Solution:

$$[A](t) = [A]_0 e^{-kt}$$

Result:

$$[A](t) = 2e^{-0.1t}$$

Here, [A](t) is the concentration of A at time t, and t is the time (in minutes).
Over time, the concentration of reactant A decreases and becomes exponentially calm.
At time 0, [A](0)=2mol/L, which is the initial condition.
At several time points
t=10min: [A](10)=0.375mol/L
t=20min: [A](20)=0.271mol/L

In conclusion, this model shows that the reaction is first order and the concentration decreases strictly exponentially with time. This example is important for the mathematical analysis of chemical reactions, helping to determine the reaction rate and the change in concentration over time.

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3. Solution depending on the order of reaction. In reaction A, the reaction is first order, and the initial concentration [A]0=2 mol/L. The reaction constant k=0.2 min-1. Find the concentration of A over time.

1) Reaction order and differential equation For a first order reaction:

$$\frac{d(A)}{dt} = -kA$$

2) We integrate in the solution:

$$\int \frac{d(A)}{dt} = -k \int dt$$

As a result:

ln[A]= − kt + C

The initial condition is [A](0) = [A]0 = 1 mol/L.

And so:ln[A]= − kt

$$[A](t) = e^{-kt}$$

Concentration with time:

$$[A](t) = 1 \times e^{-0.2t}$$

Conclusion:

Reaction order: first order

Change in concentration over time: $[A](t) = e^{0.2t}$

Solution to the problem:

- Time in 5 minutes:

$$[A](5) = e^{0.2*5}e^{-1} = 0.368 mol/L$$

- Time in 10 minutes:

$$[A](10) = e^{-2} = 0.135 mol/L$$

If the reaction is zero order, the differential equation will be:

d[A]/dt = -k

To solve this equation, we integrate:

∫ d[A] = -∫ k dt

Performing this integration, we get:

[A] = -ct + C

here:

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[A]- concentration of substance A with time change
k- reaction rate constant
t- time
C- integration constant
For example, Gaseous Decomposition (or Gas Decomposition) is zero-order. The decomposition of gas molecules as a result of a chemical reaction or physical process is zero-order, and the reaction is described as follows:

$$A \rightarrow \text{Products}$$

Conditions:
Initial concentration [A]0 = 1mol/L
The decomposition rate constant k = 0.2 mol/L
1) The differential equation of the reaction is:

$$\frac{d(A)}{dt} = -k$$

2) Solution:
We integrate: [A] = -kt + C
Initial conditions: t = 0, [A] = [A]0 = 1 mol/L

$$1 = -k \times 0 + C$$

C = 1
And so:
[A](t) = 1- 0.2t
For example:
- In 5 minutes [A](5) = 1 - 0.2·5 = 0 mol/L

Conclusion:
✓ The decay of gas molecules is zero-order, and the concentration decreases linearly with time.
✓ As time goes by, the concentration of substance A decreases steadily.

4. Chemical equilibrium and logarithmic equations.A + B⇌We use the logarithmic equation to find the equilibrium concentrations and equilibrium constant in reaction C.
Information provided:
The equilibrium concentrations of A, B, and C during the reaction are:

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[A] = 0.2 mol/L
[B] = 0.3 mol/L
[C] = 0.5 mol/L
Find the equilibrium constant K.

1) The expression for the equilibrium constant is:

Reaction: A+B⇌C
Equilibrium constant:

$$K = \frac{[C]}{[A][B]}$$

2) Calculation:

$$K = \frac{0.5}{0.2 \times 0.3} = 8.33$$

3) Logarithmic equation: A logarithmic equation is expressed in the logarithmic form of the equilibrium constant:

$$\log K = \log(\frac{0.5}{0.2 \times 0.3})$$

Let's calculate:
logK= log8.33 = 0.921

4) Conclusion:

- ✓ Equilibrium constant: K ≈ 8.33
- ✓ Logarithmic form: logK = 0.921

Chemical Equilibrium and Logarithmic Equationsis used to determine the equilibrium concentrations and equilibrium constants in chemical reaction processes. At equilibrium, the reaction rate is equal and the concentrations are constant. The equilibrium constant (K) is the ratio of the equilibrium concentrations of the products and reactants and is expressed in logarithmic form by logK. This logarithmic form is especially useful for displaying large or small values.

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REFERENCES:

1. Atkins, P., & de Paula, J. (2014). Atkins' Physical Chemistry (10th ed.). Oxford University Press.
2. Engel, T., & Reid, P. (2012). Physical Chemistry (3rd ed.). Pearson Education.
3. Espenson, J. H. (2002). Chemical Kinetics and Reaction Mechanisms (2nd ed.). McGraw-Hill.
4. Logan, J. D. (2015). Applied Mathematics (4th ed.). Wiley.
5. Levenspiel, O. (1999). Chemical Reaction Engineering (3rd ed.). Wiley.
6. Mortimer, R. G. (2008). Mathematics for Physical Chemistry (3rd ed.). Elsevier Academic Press.