The calculation of the maximum rate of oxidation of nitrogen (II) oxide using the mathematical package MathCad

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Introduction. Mathematical research methods have always been of great importance in chemistry. Mathematics allows us to build a logic model for the study of any chemical appearance that helps to better understand the chemical processes and to find qualitative and quantitative relationships between them. It is known that information about the mechanism of a chemical reaction can be obtained, in particular, by studying the rate of chemical reactions.

Materials and methods. Most chemical calculations can be made by using mathematical system MathCad, which is one of the best and most popular software products for scientific and technical computing. In MathCad are used, not artificial programming languages, a living language of mathematics: all the obtained expressions are like using only paper and pencil. The paper discusses the use of mathematical package MathCad to find the concentration of components of a gas mixture of oxygen with nitrogen (II) oxide in which the rate of formation of nitrogen (IV) oxide will be maximized.

Results. A mathematical formula which linking the reaction rate with concentrations is called the equation of the reaction rate or kinetic equation. The basic law of chemical kinetics: rate of reaction in each moment of time is proportional to the product of the concentrations of the reacting substances, elevated to the degree that represents the reaction order for that component.

As an example, consider the trimolecular reaction $2NO + O_2 = 2NO_2$ (1)

For the reaction kinetic equation will be of the form $v = \bar{k}[NO]^2[O_2]$ (2)

If to enter designations $x = \frac{[NO]}{[NO]_0}$ and $y = \frac{[O_2]}{[O_2]_0}$,where [NO] $[O_2]_0$ is the initial concentration of NO and O_2, respectively, equation (2) can be written as:

$v = kx^2 y$ (3)

where $k = \bar{k}[NO]_0[O_2]_0$

Problem statement: to determine if any oxygen content in the gas mixture the rate of oxidation of nitrogen (II) oxide will be maximized.

Solution: the concentration of NO and O_2 in equation (3) is conveniently expressed in volume percent. Then x+ y=100 and the kinetic equation takes the form

$v = k\left(100 \cdot x^2 - x^3\right)$ (4)

Thus, the challenge is to find the maximum of function (4).

For finding the maximum of the function by using MathCad. Hence y=100-66.667=33.333 the maximum O_2 concentration.

Conclusions. Thus, the calculation of this task in MathCad made it possible to find the oxygen concentration at which the reaction rate is maximum. It should be noted that this result is valid only when the reaction is irreversible, which is possible only for a particular range of temperature.