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Study of the speed of a chemical reaction involving three components

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Functions of many variables are widely used in solving mathematical problems that arise in economics [2], electromagnetic field theory, electro- and radio mechanics, heat transfer theory, theory of elasticity, hydro- and aeromechanics, etc. The feasibility of studying the functions of many variables is due to their wide use in medicine, biology, and pharmacy [1]. the work is devoted to the problem of researching the speed of a chemical reaction involving three components. In the paper, it is proposed to use partial derivatives of the second order, the function of many variables at the extremum is investigated.

A chemical reaction occurs with the participation of three substances with concentrations x, y, z. The paper examines the rate of a chemical reaction at an arbitrary moment in time $v = kx^2yz$.

The problem is: what should be the concentrations of reactants x, y, z so that the reaction rate is maximal.

The percentage concentrations of reagents satisfy the following equality:

$$x+y+z=100\%; \quad x>0;\ y>0;\ z>0.$$

From this equation we find $z=100-x-y$ and substitute in the equation for the reaction rate. We study the obtained function for extremum $v = kx^2y(100-x-y)$.

We find stationary points [2]:

$$\begin{cases} V'x = k(200xy - 3x^2y - 2xy^2) = 0 \\ V'y = k(100x^2 - x^3 - 2x^2y) = 0 \end{cases}$$

As a result, we will get two stationary points:

$(x_1;\ y_1)$=(0;0);

$(x_2;y_2)$=(50;25).

For the extremum, we examine only the point

($x_2; y_2$), because the first does not correspond to the content of the task. We find partial derivatives of the second order.

$v''_{x^2} = k(200y - 6xy - 2x^2);$ $\qquad v''_{x^2} = (50;25) = -3750k;$

$v''_{y^2} = k(-2x^2);$ $\qquad v''_{y^2} = (50;25) = -5000k;$

$v''_{xy} = k(200x - 3x^2 - 4xy);$ $\qquad v''_{xy}(50;25) = -2500k.$

The partial derivatives of the second order at the stationary point (50;25) satisfy the inequality: $v''_{z^2} \cdot v''_{y^2} - \left(v''_{xy}\right)^2 > 0$, with $v''_{x^2}(50;25) < 0.$ Therefore, according to [2], the function under study has a maximum at the stationary point (50;25).

In the results we have: at concentration x=50%; y=25%; z=25% reaction occurs at maximum speed.

The paper proposes a study of the speed of a chemical reaction using the methods of the theory of the function of many variables.

References

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