# ALGORITHM FOR SEARCHING THE OPTIMAL TEMPERATURE OF A REVERSABLE CHEMICAL REACTION

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Optimization consists in finding the extremum of the function in question or the optimal conditions for the process.

A chemical reaction is taking place. If the chemical reaction proceeds without side steps, then the reaction rate can be selected as the criterion of optimality.

$$A \underset{k_2}{\overset{k_1}{\rightleftarrows}} B$$

The objective function has the form $F = W = k_1 \cdot e^{\frac{-E_1}{RT}} \cdot C_A - k_2 \cdot e^{\frac{-E_2}{RT}} \cdot C_B$. Set limits and choose optimizing factors.

The optimality criterion $F$ depends on three parameters: $T$, $C_A$, $C_B$. But $C_A$ and $C_B$ cannot be selected as optimizing parameters, since they are not system inputs, but are reaction results, that is, to increase the speed it is necessary to have as much substance as possible $C_A$ and cannot be less $C_B$.

The goal of the process is the opposite – to increase the concentration of substance $B$ and reduce the concentration of substance $A$. Therefore, the concentrations of $C_A$ and $C_B$ cannot be considered independent factors. Thus, there is only one independent parameter that affects the function of the target $F$ – temperature. Therefore, the real problem is the problem of the optimal temperature of the chemical reaction. However, at different values $C_A$ and $C_B$ the effect of temperature can be different. Therefore, we pose the problem as follows: find the optimal temperature of the chemical reaction for fixed values $C_A$ and $C_B$:

$$\begin{cases} C_{A/t=0} = C_{A_0}; \\ C_{B/t=0} = C_{B_0}. \end{cases}$$

The second limitation of the type of inequalities (mandatory): the temperature cannot exceed a certain maximum value $T_{\max}$, $T \le T_{\max}$.

If the reaction is irreversible, that is $k_2 = 0$, then the first term remains in the equation, which grows unlimited with increasing temperature. In this case, the optimum is determined by the restriction: $T_{опт} = T_{\max}$; $W = k_1 \cdot e^{\frac{-E_1}{RT}} \cdot C_A - k_2 \cdot e^{\frac{-E_2}{RT}} \cdot C_B$; $\frac{dW}{dt} = 0$; $k_1 \cdot e^{\frac{-E_1}{RT}} \cdot C_A \cdot \frac{E_1}{R} \cdot \frac{1}{T^2} - k_2 \cdot e^{\frac{-E_2}{RT}} \cdot C_B \cdot \frac{E_2}{R} \cdot \frac{1}{T^2} = 0$. Solving this equation with respect to $T$, we obtain the optimal temperature

$$T = \frac{E_1 - E_2}{k \cdot \ln\left(\frac{E_1 \cdot k_1 \cdot C_A}{E_2 \cdot k_2 \cdot C_B}\right)}.$$