

where ΔH_T^0 , $T\Delta S$, are the changes in enthalpy and entropy at standard pressure, which can be calculated using similar formulas.

The dependence of the *Gibbs energy* on the composition of the reaction mixture reflects the *Vant-Hoff equation*:

$$\Delta G_{T,P} = \Delta G_T^0 + RT \ln P_i C_i^{v_i},$$

where R is the universal gas constant, equal to 8.314 J/mol·K;

P is a product of numbers;

C_i are concentrations of components;

v_i are the stoichiometric coefficients of the reaction equation in algebraic form:

$$\sum_i v_i A_i = 0,$$

where A_i are substances involved in the reaction (A, B, \dots, R, S, \dots);

v_i is the stoichiometric coefficient of the i -th substance.

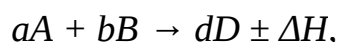
Equilibrium

The yield of the target product of the chemical-technological process is determined by the degree of approximation of the reaction system to a state of stable equilibrium, which meets the following conditions:

- invariance in time with the constancy of external conditions;
- mobility or spontaneous rebalancing after the removal of external effects;
- the dynamic nature of equilibrium due to the equalization of the rates of the direct and reverse processes;
- the ability to influence the equilibrium from both the direct and reverse reactions;
- the minimum value of the *Gibbs energy* in isobaric-isothermal processes and *Helmholtz energy* in isochoric-isothermal processes.

The degree of approach of the system to the state of stable equilibrium is characterized by a change in the isobaric-isothermal potential and the equilibrium degree of transformation. Changing the isobaric-isothermal potential ΔG determines the thermodynamic probability of the reaction under these conditions and the depth of its course.

The change in the isobaric-isothermal potential is equal to the difference between its changes for the final reaction products and the initial reagents. So, for the reaction:



$$\Delta G = d\Delta G_D - (a\Delta G_A + b\Delta G_B).$$

The sign and the order of magnitude ΔG allows to estimate the equilibrium state of the system. Thus, at values $\Delta G < 0$ the most probable is a direct reaction, and the more this inequality is, the more likely this direction of the process, at $\Delta G > 0$ the most probable is the reverse reaction, the value $\Delta G = 0$ corresponds to the equilibrium state of the system.

According to the equation:

$$\Delta G = \Delta H - T\Delta S,$$

where: ΔH and ΔS are the standard *enthalpy* and *entropy* of a system, follows that balance shift towards direct reaction is favorably influenced by great ΔH negative value (considerable thermal effect of reaction) and great ΔS positive value.