

Since entropy enters the equation in the form of a product  $T\Delta S$ , the increase in temperature increases the effect of the change in entropy.

It is obvious that the equilibrium condition ( $\Delta G = 0$ ) is equality of  $\Delta H = T\Delta S$ , that is, the influence of energy and entropy factors is equalized. At relatively low temperatures  $\Delta G \approx \Delta N$  and a characteristic of the probability of the reaction can serve as its thermal effect and the more exothermic the reaction, the more likely it is.

To assess the equilibrium state in the reactor, *an equilibrium degree of conversion* is usually used (*an equilibrium yield of the product*).

*The equilibrium degree of conversion ( $X^*$ )* is the degree of conversion of the starting materials into reaction products, corresponding to the state of stable equilibrium of the system. The equilibrium degree of conversion characterizes the depth of the process, the degree of approximation of its results to the optimum in given conditions. It is functionally related to the equilibrium constant ( $K_p$ ), and the nature of this dependence is determined by the reaction order.

For the 1st order reaction:

$$K_p = X_p^*/(1 - X_p^*) \text{ or } X_p^* = K_p/(1 + K_p),$$

for the reaction of the 2nd order:

$$K_p = 4X_p^*/(1 - X_p^*)P.$$

The relationship between the equilibrium constant and the equilibrium degree of conversion is one of the most important in chemical technology, since the latter characterizes the conditions for the maximum possible extraction of the target product from raw materials.

The shift of equilibrium towards the formation of the target product can be achieved by changing the temperature, pressure and concentration of the reactants and reaction products.

### ***Influence of temperature***

Follows from the equation of an isobar of *Vant Hoff* that as  $K=f(T)$ , and equilibrium degree of transformation of  $X^*$  depends on temperature:

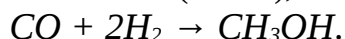
$$d\ln K/dT = \Delta H/RT^2.$$

The nature of this dependence is determined by the sign of the thermal effect of the reaction. For endothermic reactions, an increase in temperature shifts the equilibrium toward the formation of reaction products, that is, increases the equilibrium degree of conversion, and in the case of an exothermic reaction, vice versa, which is consistent with *the Le Chatelier principle*.

### ***Influence of pressure***

Pressure has a significant effect on the state of equilibrium in gaseous systems. Three cases are possible:

- the volume of the gaseous system decreases ( $\Delta V < 0$ ), for example, in the reaction:



In this case, an increase in pressure shifts the equilibrium towards the formation of reaction products;

- the volume of the gaseous system increases ( $\Delta V > 0$ ), for example, in the reaction:



In this case, the equilibrium shift towards the formation of reaction products is achieved by lowering the pressure;

- the volume of the gaseous system does not change, for example, in the reaction: