Sections 14.12 - 14.13: The Reaction Quotient (Q)

Consider the general gas phase reaction:

$$j\,A_{(g)} + k\,B_{(g)} \leftrightarrows l\,C_{(g)} + m\,D_{(g)}$$

$$K_C = \frac{[C]^l\,[D]^m}{[A]^j\,[B]^k} \quad \text{and} \quad K_P = \frac{(P_C)^l\,(P_D)^m}{(P_A)^j\,(P_B)^k}$$

For a given system at a particular temperature, the values of K_c and K_P are fixed. When the reactants and products for a given reaction are mixed, it is useful to know whether the reaction system is at equilibrium. If the system is not at equilibrium, then it is useful to know the direction in which the reaction must proceed for the system to reach equilibrium. The reaction will occur in the direction favoring either the reactants or the products.

To determine the direction in which a reaction proceeds, one needs to determine the reaction quotient, Q. Q can be expressed as Q_c or Q_P in the same way as we expressed K as K_c or K_P. For the general gas phase reaction:

$$Q_C = \frac{[C]_0^l\,[D]_0^m}{[A]_0^j\,[B]_0^k} \quad \text{and} \quad Q_P = \frac{(P_C)_0^l\,(P_D)_0^m}{(P_A)_0^j\,(P_B)_0^k}$$

Recall that $[\,]_0$ is defined as the initial concentration, and $(P)_0$ is defined as the initial partial pressure.

By comparing the numerical value of Q (Q_c or Q_P) with K (K_c or K_P), it is possible to decide the direction in which the reaction will proceed in order to achieve equilibrium.

Case 1: If $Q_c < K_c$ or $Q_P < K_P$

If Q < K, there is more reactant and less product in the initial conditions than at equilibrium. Thus, the reaction will favor the formation of products (i.e. proceed to the right) so that Q increases and eventually becomes equal to K.

Case 2: If $Q_c > K_c$ or $Q_P > K_P$

If Q > K, there is less reactant and more product in the initial conditions than at equilibrium. Thus, the reaction will favor the formation of reactants (i.e. proceed to the left) so that Q decreases and eventually becomes equal to K.

Note: **If Q = K**, the reaction system is already at equilibrium under initial conditions and there is no change.

Example: For the synthesis of ammonia at 300°C,

$$N_{2\,(g)} + 3\,H_{2\,(g)} \leftrightarrows 2\,NH_{3\,(g)} \qquad K_c = 5.2 \times 10^{-2}$$

Predict the direction in which the reaction will proceed to reach equilibrium when the initial concentrations of NH_3, N_2 and H_2 are 0.001 M, 0.0001 M, and 0.002 M, respectively.

First, calculate Q_c.

$$Q_c = \frac{[NH_3]_0^2}{[N_2]_0[H_2]_0^3}$$

$[NH_3]_0 = 0.001$ M
$[N_2]_0 = 0.0001$ M
$[H_2]_0 = 0.002$ M

$$Q_c = \frac{(0.001)^2}{(0.0001)\,(0.002)^3} = 125 \times 10^6 \qquad K_c = 5.2 \times 10^{-2}$$

Thus, $Q_c > K_c$

Q is greater than K. Hence, there is more product and less reactant in the initial conditions than at equilibrium. Thus, the reaction will proceed to the reactant side (i.e. to the left).