

13.5 - Applications of the Equilibrium Constant

The Reaction Quotient

When reactants are mixed, it is useful to know if they are at equilibrium, or if they are not, the direction in which the system must shift to reach equilibrium.

The Reaction Quotient concept is used for this: it is obtained by using *initial concentrations* in the equilibrium concentration expression.

For example, in the synthesis of ammonia,

$N_{2(g)} + 3H_{2(g)} \rightleftharpoons 2NH_{3(g)}$
the quotient would be calculated thusly:

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

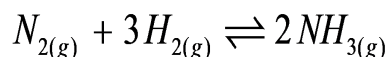
Note: subscripted zeros denote initial concentrations.

Quotient Results

When initial concentrations are used to find Q , three outcomes are possible:

1. $Q = K$. It's at equilibrium - no shift occurs.
2. $Q > K$. Ratio of initial products to reactants is too large. Reaction shifts to the left - consuming products and forming reactants.
3. $Q < K$. Ratio of initial products to reactants is too small. Reaction shifts to the right - forming more products.

Quotient Examples



At 500°C, K for ammonia synthesis is 6.0×10^{-2} .

Predict the direction that the system will shift for the following concentrations:

Problem	[NH ₃]	[N ₂]	[H ₂]
1	1.0 E-3	1.0 E-5	2.0 E-3
2	2.0 E-4	1.5 E-5	3.54 E-1
3	1.0 E-4	5.0	1.0 E-2

Quotient Answers

1. Using the equilibrium expression for ammonia:

$$K = \frac{[NH_3]_0^2}{[N_2]_0[H_2]_0^3} = \frac{(1.0E-3)^2}{(1.0E-5)(2.0E-3)^3} = \boxed{1.3E7}$$

Since Q is greater than K , this reaction will shift to the left, forming reactants until equilibrium is reestablished.

2. Plugging in values again:

$$K = \frac{[NH_3]_0^2}{[N_2]_0[H_2]_0^3} = \frac{(2.0E-4)^2}{(1.5E-5)(3.54E-1)^3} = \boxed{6.0E-2}$$

This is at equilibrium, $Q = K$.

3. Once more, with feeling!

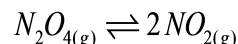
$$K = \frac{[NH_3]_0^2}{[N_2]_0[H_2]_0^3} = \frac{(1.0E-4)^2}{(5.0)(1.0E-2)^3} = \boxed{2.0E-3}$$

This favors more products.

4. Calculating Pressures I

Many equilibrium problems involve finding equilibrium concentrations of reactants and products, given the initial concentrations and K . These problems can become complicated mathematically, but some strategies are laid out in the following examples.

Dinitrogen tetroxide decomposes into nitrogen dioxide:



If $K_p = 0.133$, and the pressure of N_2O_4 at equilibrium is 2.71 atm, calculate the equilibrium pressure of NO_2 .

4. Calculating Pressures I Solution

Using the equilibrium expression for this reaction, and our known quantities, we get the answer:

$$K_p = \frac{P_{NO_2}^2}{P_{N_2O_4}}$$

$$K_p \cdot P_{N_2O_4} = P_{NO_2}^2$$

$$P_{NO_2} = \sqrt{K_p \cdot P_{N_2O_4}} = \sqrt{0.133 \cdot 2.71} = \boxed{0.600 \text{ atm}}$$

5. Calculating Eq. Pressures II

A 1.00 L flask initially contained 0.298 mol PCl_5 , and 8.70×10^{-3} mol PCl_3 . After the system reaches equilibrium, 2.00×10^{-3} moles Cl_2 was found in the flask. The reaction is:



Calculate the equilibrium concentrations of all species, and the value of K .

5. Eq. Pressures II Solution

Using the ratios of reactants: 1 : 1 : 1 is the key.

First, since 2.00×10^{-3} moles of chlorine was produced, 2.00×10^{-3} moles PCl_5 decomposed. Thus:

$$PCl_{5(g)} = 8.70 \times 10^{-3} \text{ mol} - 2.00 \times 10^{-3} \text{ mol} = 6.70 \times 10^{-3} \text{ mol } PCl_{5(g)}$$

Next, an additional 2.00×10^{-3} moles of PCl_3 must have formed as well:

$$PCl_{3(g)} = 0.298 \text{ mol} + 2.00 \times 10^{-3} \text{ mol} = 0.300 \text{ mol } PCl_{3(g)}$$

We can now calculate molar concentrations, all in the 1.00 L flask (this would be more complex if it were any other volume):

$$[PCl_5] = 6.70 \times 10^{-3} \text{ M};$$

$$[PCl_3] = 0.300 \text{ M};$$

$$[Cl_2] = 2.00 \times 10^{-3} \text{ M}.$$

5. Eq. Pressures II Solution

Finally, we calculate K :

$$K = \frac{[PCl_3][Cl_2]}{[PCl_5]} = \frac{(0.300)(2.00 \times 10^{-3})}{6.70 \times 10^{-3}} = \boxed{8.96 \times 10^{-2}}$$

Note, if the flask had been any other volume, this K would be different. Volume matters!

If this mixture were in a small volume, pressure would be increased, and equilibrium conditions would change - we'll see this later as Le Chatelier's principle.

6. What is the hypothetical K , if the flask were 2.0 L? Effectively, this halves all concentrations:

$$K' = \frac{\frac{1}{2} \cdot \frac{1}{2}}{\frac{1}{2}} = \frac{1}{2} K = \frac{1}{2} \cdot 8.96 \times 10^{-2} = \boxed{4.48 \times 10^{-2}}$$

Homework

Preview 12.6

13.5 Problems in your Booklet
Due: Next Class