Equilibrium I: Basic Principles and Calculations

Remember the important associations about mass actions and equilibrium constant expressions:

✓**Reverse the direction the equation is written**	→	**invert *K***
✓**Add chemical equations**	→	**multiply the *K*'s for the reactions**
✓**Increase stoichiometric coefficients by a factor**	→	**raise *K* to the power of factor**

1. What is the calculated K_c for

$$2\,H_{2(g)} + O_{2(g)} \rightleftarrows 2\,H_2O_{(g)}$$

given the the following reactions:

$$CO_2(g) + H_2(g) \rightleftarrows CO(g) + H_2O(g) \quad K_c = 1.4$$
$$C(s) + \tfrac{1}{2}O_2(g) \rightleftarrows CO(g) \quad K_c = 1.0 \times 10^8$$
$$C(s) + CO_2(g) \rightleftarrows 2\,CO(g) \quad K_c = 0.64$$

$$2\,CO_2(g) + 2\,H_2(g) \rightleftarrows 2\,CO(g) + 2\,H_2O(g) \quad K_c = (1.4)^2 = 1.96$$
$$2\,C(s) + O_2(g) \rightleftarrows 2\,CO(g) \quad K_c = (1.0 \times 10^8)^2 = 1 \times 10^{16}$$
$$4\,CO(g) \rightleftarrows 2\,C(s) + 2\,CO_2(g) \quad K_c = [(0.64)^2]^{-1} = 2.44$$

$$2\,H_{2(g)} + O_{2(g)} \rightleftarrows 2\,H_2O_{(g)} \quad K_c = 1.96 \times (1 \times 10^{16}) \times 2.44 = 4.8 \times 10^{16}$$

2. For the reaction:

$$COCl_2(g) \rightleftarrows CO(g) + Cl_2(g) \quad K_c = 8.3 \times 10^{-4}\ (395°C)$$

a. What direction will the reaction proceed if 0.100 mol of $COCl_2$ is placed in a 2.0 L container and heated to 395°C?

Since no products are introduced into the container, the reaction *must* proceed to the right.

b. What direction will the reaction proceed if 0.030 mol of each gas are placed in a 2.0 L vessel and heated?

$$Q = \frac{[CO][Cl_2]}{[COCl_2]} = \frac{\left(0.030\text{ mol}/2.0\text{ L}\right)\left(0.030\text{ mol}/2.0\text{ L}\right)}{\left(0.030\text{ mol}/2.0\text{ L}\right)} = 0.015$$

$Q > K$ so reaction proceeds to the left.

c. For question a, what is the final concentration of each gas?

$$8.3\times10^{-4} = \frac{x \cdot x}{0.050 - x}$$ now solve this either by the quadratic formula, numerically by successive approximations, or with a "solver".

$x = [CO] = [Cl_2] = 0.0060\text{ M}$

$[COCl_2] = 0.050\text{ M} - 0.0060\text{ M} = 0.044\text{ M}$

d. For question b, what is the final concentration of each gas?

$$8.3\times10^{-4} = \frac{(0.015 - x)(0.015 - x)}{0.015 + x}$$ now solve this either by the quadratic formula, numerically by successive approximations, or with a "solver".

x = the change in concentrations = 0.0104 M

$[CO] = [Cl_2] = 0.015\text{ M} - 0.0104\text{ M} = 0.0046\text{ M}$

$[COCl_2] = 0.015\text{ M} + 0.0104\text{ M} = 0.025\text{ M}$

3. A quantity of 0.10 mol of I_2 and 0.10 mol H_2 are placed in a 1.00-L reaction vessel at 430°C. Calculate the equilibrium concentration of all species after equilibrium has been established.

$$H_2(g) + I_2(g) \rightleftarrows 2\,HI(g) \qquad K_c = 54.3$$

$$K_c = \frac{[HI]^2}{[H_2][I_2]}$$

Let x be the decrease in each reactant concentration and $2x$ be the increase in product concentration:

$$54.3 = \frac{(2x)^2}{(0.10\text{ M} - x)(0.10\text{ M} - x)}$$

Use any suitable method to solve the equation. Notice that the equation can be easily simplified so that it is not a quadratic.

$x = 0.0787$ M

$[H_2] = [I_2] = 0.10\text{ M} - 0.0787\text{ M} = 0.021\text{ M}$

$[HI] = 2 \times 0.0787\text{ M} = 0.16\text{ M}$

4. The K_c for the reaction

$$N_2(g) + 3\,H_2(g) \rightleftarrows 2\,NH_3(g)$$

At 300°C is 0.45. Predict whether the reaction will proceed to the right, left, or is already at equilibrium when 0.10 mol N_2, 0.30 mol H_2, and 0.2 mol NH_3 are placed in a 2.00-L container and heated to 300°C. If a reaction occurs, what is the final concentration of each species?

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

$$Q = \frac{(0.1\text{ M})^2}{(0.05\text{ M})(0.15\text{ M})^3} = 59 \quad Q > K \text{ so reaction proceeds to the left}$$

$$0.45 = \frac{(0.1\text{ M} - 2x)^2}{(0.05\text{ M} + x)(0.15\text{ M} + 3x)^3} \quad x = 0.0369\text{ M}$$

$[N_2] = 0.05\text{ M} + 0.0369\text{ M} = 0.087\text{ M}$

$[H_2] = 0.15\text{ M} + 3(0.0369\text{ M}) = 0.261\text{ M}$

$[NH_3] = 0.1\text{ M} - 2(0.0369\text{ M}) = 0.026\text{ M}$

5. The following quantities of reagents are introduced into a 1.00-L reaction vessel: 0.15 mol H_2, 0.23 mol I_2, and 0.015 mol HI. The reaction vessel is then thermostatted at 430°C. Convince yourself that the system is not at equilibrium and will shift right (to produce more product). What are the equilibrium concentrations of all species? (See problem 3 for additional information.)

$$K_c = \frac{[\mathrm{HI}]^2}{[\mathrm{H_2}][\mathrm{I_2}]}$$

$$Q = \frac{(0.015\ \mathrm{M})^2}{(0.15\ \mathrm{M})(0.23\ \mathrm{M})} = 0.0065 \quad Q < K;\ \text{reaction proceeds right}$$

$$54.3 = \frac{(0.015\ \mathrm{M} + 2x)^2}{(0.15\ \mathrm{M} - x)(0.23\ \mathrm{M} - x)}$$

Use any suitable method to solve the equation.

$$x = 0.134\ \mathrm{M}$$

$$[\mathrm{H_2}] = 0.15\ \mathrm{M} - 0.134\ \mathrm{M} = 0.016\ \mathrm{M}$$

$$[\mathrm{I_2}] = 0.23\ \mathrm{M} - 0.134\mathrm{M} = 0.096\ \mathrm{M}$$

$$[\mathrm{HI}] = 0.015\ \mathrm{M} + 2 \times 0.134\ \mathrm{M} = 0.284\ \mathrm{M}$$

6. For question 5, what will be the effect on the equilibrium concentrations if the volume of the container is reduced to 500.0 mL with no loss of reagents.

7. Consider the system at equilibrium in problem 4: what will be the new equilibrium concentrations if the volume of the container is reduced to 1.00 L with no loss of reactants or products?

$[N_2] = 0.087\ \text{M} \qquad [H_2] = 0.261\ \text{M} \qquad [NH_3] = 0.026\ \text{M}$

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

All initial concentrations double since volume is halved:

$$Q = \frac{(0.052\ \text{M})^2}{(0.174\ \text{M})(0.522\ \text{M})^3} = 0.109 \quad Q < K \text{ so reaction proceeds to the right}$$

This could be predicted without calculating Q by realizing that the concentrations will increase (by ratio) more on the left than right.

$$0.45 = \frac{(0.052\ \text{M} + 2x)^2}{(0.174\ \text{M} - x)(0.522\ \text{M} - 3x)^3} \quad x = 0.0170\ \text{M}$$

$[N_2] = 0.174\ \text{M} - 0.017\ \text{M} = 0.157\ \text{M}$

$[H_2] = 0.522\ \text{M} - 3(0.017\ \text{M}) = 0.471\ \text{M}$

$[NH_3] = 0.052\ \text{M} + 2(0.017\ \text{M}) = 0.086\ \text{M}$

8. Consider the system at equilibrium in problem 4: what will be the new equilibrium concentrations if the total pressure in the container is increased by adding 1.0 atm of helium gas?

The partial pressures of the reactants and products remains unchanged so nothing happens.