

CHEMICAL EQUILIBRIUM CALCULATIONS

4.13 Team 1

16

CALCULATING K_p FOR A HOMOGENEOUS GAS-PHASE EQUILIBRIUM

Homogeneous means everything is in the same phase – i.e. all chemicals are gases here

Chemical	N_2	O_2	NO
Moles at equilibrium	0.950	0.950	0.100
Mole fractions	0.475	0.475	0.050
Partial pressure (atm)	$p(N_2) = 23.75$	$p(O_2) = 23.75$	$p(NO) = 2.50$

Mole fraction $\times 50$ atm

Nitrogen and oxygen can react to form an equilibrium mixture with nitrogen monoxide: $N_{2(g)} + O_{2(g)} \rightleftharpoons 2NO_{(g)}$. The equilibrium was set up in a sealed container at a pressure of 50 atm. Analysis of the equilibrium mixture found its composition to be as shown in the table.

$$K_p \text{ can be calculated from the partial pressures like this: } K_p = \frac{p(NO)^2}{p(N_2)p(O_2)} = \frac{2.50^2}{23.75 \times 23.75} = 0.0111$$

In this case there are no units for K_p because they cancel: $K_p = \frac{\text{atm}^2}{\text{atm} \times \text{atm}}$

EXAM TIP
Always work out the units like this

Example 1

- a) Phosgene is produced via the following reaction: $CO_{(g)} + Cl_{2(g)} \rightleftharpoons COCl_{2(g)}$. In one experiment, 0.450 moles of CO were mixed with 0.550 moles of Cl_2 and allowed to reach equilibrium at 25 °C and 101 kPa, and 0.395 moles of phosgene formed. Calculate K_p .

	CO	Cl_2	$COCl_2$
Initial amount (moles)	0.450	0.550	0
Change (moles)	-0.395	-0.395	+0.395
Equilibrium amount (moles)	0.055	0.155	0.395
Mole fraction, x	0.091	0.256	0.653

$$p(CO) = x(CO) \times P = 0.091 \times 101 \text{ kPa} = 9.2 \text{ kPa}$$

$$p(Cl_2) = x(Cl_2) \times P = 0.256 \times 101 \text{ kPa} = 25.9 \text{ kPa}$$

$$p(COCl_2) = x(COCl_2) \times P = 0.653 \times 101 \text{ kPa} = 66.0 \text{ kPa}$$

$$K_p = \frac{p(COCl_2)}{p(CO)p(Cl_2)} = \frac{66.0 \text{ kPa}}{9.2 \text{ kPa} \times 25.9 \text{ kPa}} = 0.277 \text{ kPa}^{-1}$$

EXAM TIP
The units of K_p are not the same in all calculations – work them out every time

- b) The enthalpy change for the reaction is -110 kJ mol^{-1} . If the equilibrium mixture were heated, would this improve the yield of phosgene? Explain your answer.

No – because the reaction is exothermic, K_p would decrease (the position of equilibrium would move left) and less phosgene would be in the equilibrium mixture at a higher temperature.

Example 2

- a) Methanol can be formed from this reaction: $CO_{(g)} + 2H_{2(g)} \rightleftharpoons CH_3OH_{(g)}$. When 1.365 moles of CO were mixed with 2.550 moles of H_2 and allowed to reach equilibrium at 25 °C in a 2.000 dm³ container, 1.095 moles of CO were found in the mixture. Calculate K_c .

	CO	H_2	CH_3OH
Initial amount (moles)	1.365	2.550	0
Change (moles)	-0.270	-0.540	+0.270
Equilibrium amount (moles)	1.095	2.010	0.270
Concentration (mol dm ⁻³)	0.5475	1.005	0.135

1 : 2 reacting ratio

1.095 mol/2.000 dm³

$$K_c = \frac{[CH_3OH]}{[CO][H_2]^2} = \frac{0.135 \text{ mol dm}^{-3}}{0.5475 \text{ mol dm}^{-3} \times (1.005)^2 \text{ mol}^2 \text{ dm}^{-6}} = 0.244 \text{ mol}^2 \text{ dm}^{-4}$$

$2H_2$ in equation

- b) More H_2 was added to the mixture. The temperature remained constant. How would this affect:
- The position of equilibrium
 - the value of K_c ?

- The position of equilibrium would move to the right;
- The value of K_c would be unchanged

EXAM TIP

If the question says that the temperature does not change, it is a clue that K_c has not changed