CHEM 102 Class 5

Writing ICE tables

(1) Write an ICE table (but don't solve it) for 1.0 M SO_3 reacting with 2.0 M H_2O according to the equation $SO_3(g) + H_2O(g)$ _ $H_2SO_4(g)$

	$SO_3(g)$	+ $H_2O(g)$	_ $H_2SO_4(g)$
Initial	1.0 M	2.0 M	0
Change	- x	- x	+ x
Equilibrium	1.0 - x	1.0 - x	x

(2) Write an ICE table (but don't solve it) for 0.66 atm H_2 reacting with 1.28 atm O_2 according to the equation $2 H_2(g) + O_2(g)$ _ $2 H_2O(g)$

	$2 H_2(g)$	+ $O_2(g)$	_ $2 H_2O(g)$
Initial	0.66 atm	1.28 atm	0
Change	- 2x	- x	+ 2x
Equilibrium	0.66 - 2x	1.28 - x	2x

(3) In a container of 10.0 L volume, I mix 1.0 mol N_2, 1.0 mol H_2 and 0.5 mol O_2. Write an ICE table (but don't solve it) for the equilibrium $N_2(g) + 4 H_2(g) + O_2(g)$ _ $N_2H_4(g) +$ $2 H_2O(g)$

The initial concentrations of the gases are N_2 = 1.0 mol / 10.0 L = 0.1 M, H_2 = 1.0 mol / 10.0 L, O_2 = 0.5 mol / 10.0 L = 0.05 M

	$N_2(g)$	+ 4 $H_2(g)$	$O_2(g)$	_ $N_2H_4(g)$	+ 2 $H_2O(g)$
Initial	0.1 M	0.1 M	0.05 M	0	0
Change	- x	- 4x	- x	+ x	+ 2x
Equilibrium	0.1 - x	0.1 - 4x	0.05 - x	x	2x

Solving equilibrium problems – finding K

(4) In the reaction $2\,NO_2(g)\_N_2O_4(g)$ the initial concentration of N_2O_4 was 0.100 M and NO_2 was 0.000 M. At equilibrium, the concentration of N_2O_4 was measured as 0.009 M. Calculate K_c.

First set up an ICE table

	NO$_2$	N$_2$O$_4$
Initial	0.000	0.100
Change	+2x	-x
Equilibrium	0.000 + 2x	0.009

We can see from the last column that x must be 0.100 M – 0.009 M = 0.091 M. We can now calculated the equilibrium value of NO_2 as 0.000 + (2 x 0.091) = 0.182 M. Hence the value for K_c is

$$K_c = \frac{[N_2O_4]}{[NO_2]^2} = \frac{0.009\ M}{0.182\ M^2} = 0.27$$

(5) In the reaction $2\,NO_2(g)\_N_2O_4(g)$ the initial concentration of NO_2 was 0.250 M and N_2O_4 was 0.000 M. At equilibrium, the concentration of N_2O_4 was measured as 0.0133 M. (a) Calculate the equilibrium concentration of NO_2 (b) Calculate K_c.

First set up an ICE table

|	NO$_2$	N$_2$O$_4$
Initial	0.250	0.000
Change	-2x	+x
Equilibrium	0.250 - 2x	0.0133

We can see from the last column that x must be 0.0133 M.

(a) We can now calculate the equilibrium value of NO_2 as 0.250 – 2x = 0.250 – 0.0266 = 0.2234 M

(b) Hence the value for K_c is

$$K_c = \frac{[N_2O_4]}{[NO_2]^2} = \frac{0.0133\ M}{0.2234\ M^2} = 0.27$$

Notice that the initial composition was very different than in (4), that the equilibrium amounts of the gases are different but K_c is the same! It doesn't matter whether you start with reactants, as in (4), or products, as in (5), the same value of K is reached at equilibrium.

(6) Initially, a mixture of 0.100 M NO, 0.050 M H_2 and 0.100 M H_2O was allowed to reach equilibrium. There was no N_2 present initially. At equilibrium, the concentration of NO was found to be 0.062 M. Calculate K_c.

$$2\ NO(g) + 2\ H_2(g) \ \_ \ N_2(g) + 2\ H_2O(g)$$
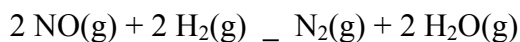
	NO	H_2	N_2	H_2O
Initial	0.100 M	0.050 M	0.000 M	0.100 M
Change	- 2x	- 2x	+x	+ 2x
Equilibrium	0.062 M			

Note the change in the NO concentration was (0.100 M – 0.062 M) = 0.038 M. This represents a decrease of 2x so x = 0.019. Now we know x, we can complete the ICE table

	NO	H_2	N_2	H_2O
Initial	0.100 M	0.050 M	0.000 M	0.100 M
Change	-0.038 M	-0.038 M	+0.019 M	+0.038 M
Equilibrium	0.062 M	0.012 M	0.019 M	0.138 M

Finally, we can calculate K_c

$$K_c = \frac{[N_2]\cdot[H_2O]^2}{[NO]^2\cdot[H_2]^2} = \frac{[0.019]\cdot[0.138]^2}{[0.062]^2\cdot[0.012]^2} = 650$$

Solving equilibrium problems – given K

(7) In the following reaction, $K_p = 9.3 \times 10^{-7}$ at room temperature. Calculate the equilibrium concentration of N_2O_4 in a flask initially containing only 3.00 atm of NO_2

$$2\ NO_2(g) \ \_ \ N_2O_4(g)$$
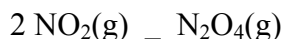
	NO_2	N_2O_4

Initial	3.00 atm	0.00 atm
Change	- 2x	+x
Equilibrium	3.00 – 2x	x

Insert into the expression for K_p

$$K_p = \frac{p(N_2O_4)}{p(NO)^2} = \frac{x}{(3.00 - 2x)^2} = 9.3\times10^{-7}$$

Because K_p is very small, we expect the concentration of N_2O_4 to be very small compared with the concentration of NO_2 and we can set $3.00 - 2x = 3.00$.
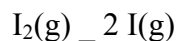
$$K_p = \frac{x}{(3.00)^2} = 9.3\times10^{-7}$$

$$x = 8.4\times10^{-6} \text{ atm}$$

Check to see if x is less than 5% of the initial value, $(8.4\times10^{-6}$ atm / 3.00 atm) x 100 = 2.8×10^{-4}% - assumption OK

Check the value of $K_p = 8.4\times10^{-9} / 3.00^2 = 9.33\times10^{-7}$

(8) Iodine molecules dissociate at high temperature according to the reaction

$$I_2(g) \_ 2\ I(g)$$

If $K_p = 4.5\times10^{-4}$ and the reaction initially starts with only I_2 with a pressure of 1.000 atm, what is the pressure of (a) $I_2(g)$ and (b) $I(g)$ at equilibrium?

	$I_2(g)$	$I(g)$
Initial	1.000	0.000
Change	-x	+2x
Equilibrium	1.000 - x	2x

Insert into the expression for K_p

$$K_p = \frac{p(I)^2}{p(I_2)}$$

$$4.5x10^{-4} = \frac{(2x)^2}{1.000 - x}$$

$$1.00 - x \cdot (4.5x10^{-4}) = 4x^2$$

$$4.5x10^{-4} - 4.5x10^{-4}x = 4x^2$$

$$4.5x10^{-4} = 4x^2 + 4.5x10^{-4}x$$

$$0 = 4x^2 + 4.5x10^{-4}x - 4.5x10^{-4}$$

This is a quadratic equation with solutions x = 0.0105 or -0.0106. The negative solution must be incorrect) otherwise the equilibrium concentration of I(g) would be negative).

(a) The pressure of I_2 at equilibrium is 1.000 atm – 0.0105 atm = 0.989 atm

(b) The pressure of I at equilibrium is 2x = 0.021 atm

(9) 0.05 mol H_2(g) and and 0.05 mol Br_2(g) are placed together in a 5.0 L flask and heated to 700 K. What is the concentration of each substance in the flask at equilibrium if K_c = 64 at 700 K?

$$H_2(g) + Br_2(g) \,\_\, 2\ HBr(g)$$
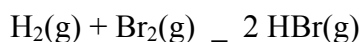
The initial concentrations are $[H_2]$ = $[Br_2]$ = 0.05 mol / 5.0 L = 0.01 M and $[HBr]$ = 0.

	H_2(g)	Br_2(g)	HBr(g)
Initial	0.01 M	0.01 M	0
Change	- x	- x	+ 2x
Equilibrium	0.01 - x	0.01 - x	2x

Insert into the equilibrium expression, assume that x is small in the denominator and solve

$$K_c = \frac{[HBr]^2}{[H_2] \cdot [Br_2]} = \frac{(2x)^2}{(0.01 - x) \cdot (0.01 - x)} \approx \frac{4x^2}{0.01 \cdot 0.01} = 64$$

$$4x^2 = 64 \cdot 0.0001$$

$$= 0.0064$$

$$x = \sqrt{\frac{0.0064}{4}} = 0.04$$

Check that 0.04 is small (<5%) compared with the initial concentrations: (0.04 / 0.01) x 100 = 400%. The "x is small" assumption is clearly false here and we must solve a quadratic equation.

$$K_c = \frac{[HBr]^2}{[H_2] \cdot [Br_2]} = \frac{(2x)^2}{(0.01-x) \cdot (0.01-x)} = \frac{4x^2}{0.0001 - 0.02x + x^2} = 64$$

$$4x^2 = 64 \cdot \left(0.0001 - 0.02x + x^2\right)$$

$$= 0.0064 - 1.28x + 64x^2$$

$$0 = 60x^2 - 1.28x + 0.0064$$

Using the quadratic equation solving formula produces two solutions for x (0.008 and 0.0133). Clearly the last one is inappropriate here (0.01 – x would give a negative concentration) so the answer must be 0.008 M.

Therefore, the concentrations are [H$_2$] = [Br$_2$] = 0.01 M – 0.008 M = 0.002 M and [HBr] = 2x = 0.016 M

Check K$_c$ = (0.016)^2 / (0.002 x 0.002) = 64

(10) A mixture consisting of 3.00 mols H$_2$O$_2$, 2.00 mols O$_2$ and 5.00 mols of H$_2$ in a 5.00 L container was heated to 900 K and allowed to reach equilibrium. Determine the equilibrium amounts of each substance if K$_c$ = 0.0076 at 900 K.

$$H_2O_2(g) \;\rule[0.5ex]{1em}{0.4pt}\; O_2(g) + H_2(g)$$
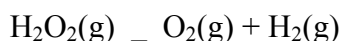
Initial concentrations [H$_2$O$_2$] = 3.00 mols / 5.00 L = 0.600 M, [O$_2$] = 2.00 mols / 5.00 L = 0.400 M, [H$_2$] = 5.00 mols / 5.00 L = 1.000 M

	H$_2$O$_2$(g)	O$_2$(g)	H$_2$(g)
Initial	0.600 M	0.400 M	1.000 M
Change	?	?	?
Equilibrium	?	?	?

We do not yet know whether we are moving towards equilibrium (in which case [H$_2$O$_2$] will decrease) or whether we are past equilibrium (in which case [H$_2$O$_2$] will increase.

Calculating Q

$$Q_c = \frac{[O_2] \cdot [H_2]}{[H_2O_2]} = \frac{(0.4) \times (1.0)}{0.6} = 0.67$$

Since Q is greater than K we are past equilibrium and as we move towards it we will decrease the product concentrations and increase the reactant

	$H_2O_2(g)$	$O_2(g)$	$H_2(g)$
Initial	0.600 M	0.400 M	1.000 M
Change	+ x	- x	- x
Equilibrium	0.600 + x	0.400 – x	1.000 – x

$$K_c = \frac{[O_2] \cdot [H_2]}{[H_2O_2]} = \frac{(0.4 - x) \times (1 - x)}{(0.6 + x)} = 0.0076$$

$$(0.4 - x) \times (1 - x) = 0.0076 \cdot (0.6 + x)$$

$$0.4 - 1.4x + x^2 = 0.00456 + 0.0076x$$

$$x^2 - 1.4076x + 0.395 = 0$$

Solving this gives x = 1.02 or 0.387. Clearly the first answer is inappropriate so x = 0.387. Hence, the concentrations at equilibrium are $[H_2O_2]$ = 0.6 + 0.39 = 0.99 M, $[O_2]$ = 0.4 – 0.39 = 0.01 M and $[H_2]$ = 1 – 0.39 = 0.61 M.

Check K_c = 0.01 x 0.61 / 0.99 = 0.0062 (close to 0.0076 with rounding errors)