Equilibrium Calculations

1. Calculating K_{eq} from equilibrium concentrations:

Consider the following equilibrium system:

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

At 200°C, the concentrations of nitrogen, hydrogen and ammonia at equilibrium are measured and found to be $[N_2] = 2.12$, $[H_2] = 1.75$ and $[NH_3] = 84.3$. Determine the value of K_{eq}.

$$Keq = \frac{[NH_3]^2}{[N_2][H_2]^3} = \frac{(84.3)^2}{(2.12)(1.75)^3}$$

$$= 625$$

2. Calculating concentrations from K_{eq}:

The equilibrium concentrations of SO_2 and O_2 are each 0.0500M and $K_{eq} = 85.0$ at 25°C for the reaction:

$$2SO_2(g) + O_2(g) \rightleftarrows 2SO_3(g)$$

Calculate the equilibrium concentration for SO_3 at this temperature.

$$Keq = \frac{[SO_3]^2}{[SO_2]^2[O_2]}$$

$$[SO_3]^2 = (Keq)[SO_2]^2[O_2]$$

$$[SO_3]^2 = (85.0)(0.05)^2(0.05)$$

$$[SO_3]^2 = 0.010625 \qquad [SO_3]_{eq} = \underline{0.103M}$$

3. Calculating K_{eq} from initial concentrations:

Suppose that 4.00 moles of HI(g) is placed into a 2.00 L flask at 425°C and reacts to produce H_2 and I_2 according to the equation:

$$2HI(g) \rightleftarrows H_2(g) + I_2(g)$$

At equilibrium the concentrations of H_2 and I_2 are found to each be 0.214 mol/L. Calculate the value of K_{eq}.

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

* Don't need x - put in #s !!

$[HI]_{initial} = \frac{4.00 \text{ mol}}{2.00 \text{ L}} = 2.00 \frac{\text{mol}}{\text{L}}$

$[H_2]_{eq} = [I_2]_{eq} = 0.214 \text{ M}$

⇒ create an ICE table

	$2HI_{(g)}$ ⇌	$H_{2(g)}$ +	$I_{2(g)}$
Initial	2.00 M	0.00 M	0.00 M
change	$-2x$	$+x$	$+x$
equilibrium	$2-2x$	x	x

@ equilib $x = [H_2] = [I_2] = 0.214 \text{ M}$

$[HI] = 2 - 2(.214) = 1.57 \text{ M}$

$K_{eq} = \frac{(0.214)(0.214)}{(1.57)^2} = 1.86 \times 10^{-2}$

4. Calculating initial concentrations from K_{eq}:

A certain amount of $NO_2(g)$ was placed into a 5.00L bulb and reacted according to the equation:

$$2NO(g) + O_2(g) \rightleftarrows 2NO_2(g)$$

When equilibrium was reached, the concentration of NO(g) was 0.800 M. If K_{eq} has a value of 24.0, how many moles of NO_2 were originally placed into the bulb?

$K_{eq} = \frac{[NO_2]^2}{[NO]^2[O_2]}$

$[NO]_{eq} = 0.800M$

$[NO_2]_{initial} = y$

	$2NO_{(g)}$ +	$O_{2(g)}$ ⇄	$2NO_{2(g)}$
I	0	0	y
C	+2x	+x	-2x
E	2x	x	y-2x

$2x = 0.800M$

$x = 0.400M$

$y - 0.800M$

$K_{eq} = \frac{[NO_2]^2}{[NO]^2[O_2]}$

$24.0 = \frac{(y-0.800)^2}{(.800)^2(.400)}$

$24.0 = \frac{(y-0.800)^2}{0.256}$

$(y-0.800)^2 = (24.0)(.256)$

$(y-0.800)^2 = 6.144$

$y - 0.800 = 2.479$

$y = 3.279M$ $[NO_2]_{initial}$

moles NO_2 = $(3.279\frac{mol}{L})(5.00L)$

$= \boxed{16.4\ mol}$

5. Determining [equilibrium] from [initial]

$K_{eq} = 3.5$ for the reaction:

$$SO_2(g) + NO_2(g) \rightleftarrows SO_3(g) + NO(g)$$

If 4.0 mol of $SO_2(g)$ and 4.0 mol of $NO_2(g)$ are put into a 5.0 L bulb and allowed to come to equilibrium, what concentration of all species will exist at equilibrium?

$K_{eq} = \frac{[SO_3][NO]}{[SO_2][NO_2]}$

	$SO_{2(g)}$ +	$NO_{2(g)}$ $\rightleftarrows$	$SO_{3(g)}$ +	$NO_{(g)}$
I	0.80M	0.80M	0	0
C	$-x$	$-x$	$+x$	$+x$
E	$0.80-x$	$0.80-x$	x	x

initial

$[SO_2] = [NO_2] = \frac{4.0\ mol}{5.0\ L} = 0.80M$

$K_{eq} = 3.5 = \frac{x^2}{(.80-x)}$

$1.87 = \frac{x}{.8-x}$

$1.87(.8-x) = x$

$1.496 - 1.87x = x$

$1.496 = 2.87x$

$x = 0.52M$

@ equilib

$[SO_3] = 0.52M$

$[NO] = 0.52M$

$[SO_2] = 0.28M$

$[NO_2] = 0.28M$

6. Determining [equilibrium] after a shift

A 1.0 L reaction vessel contained 1.0 mol of SO_2, 4.0 mol of NO_2, 4.0 mol of SO_3 and 4.0 mol of NO at equilibrium according to the reaction:

$$SO_2(g) + NO_2(g) \rightleftarrows SO_3(g) + NO(g)$$

If 3.0 mol of SO_2 are added to the mixture, what will the new concentration of NO be when equilibrium is re-established?

$K_{eq} = \frac{[SO_3][NO]}{[SO_2][NO_2]} = \frac{(4.0)(4.0)}{(1.0)(4.0)} = 4.0$

	SO_2	$+ NO_2$	$\rightleftharpoons SO_3$	$+ NO$
I	1.0 + 3.0	4.0	4.0	4.0
C	$-x$	$-x$	$+x$	$+x$
E	$4.0-x$	$4.0-x$	$4.0+x$	$4.0+x$

$K_{eq} = \frac{(4.0+x)^2}{(4.0-x)^2} = 4.0$

$\frac{4.0+x}{4.0-x} = 2.0$

$4.0+x = 2(4.0-x)$

$4.0+x = 8.0 - 2.0x$

$3.0x = 4.0$

$x = 1.33\,M$

$[NO] = 4.0 + 1.33$

$= \boxed{5.3\,M}$

- for some problems, a numerical answer is NOT required but rather a DECISION must be made
  - > for example . . . which way will the reaction shift in order to reach equilibrium? OR
  - > how will the concentration of reactants and products change in order to reach equilibrium?
- for these decision type problems a **reaction quotient (Q)** or **Trial K_{eq}** is used

Consider the following equation:

$$2NO(g) + O_2(g) \rightleftarrows 2NO_2(g)$$

the reaction quotient is:

$$Q = \frac{[NO_2]^2}{[NO]^2[O_2]}$$

- notice that the reaction quotient is the same as the equilibrium expression except that we will use initial concentrations to solve for Q
- our decision will be based on comparing the reaction quotient (Q) to the equilibrium constant (K_{eq})

If $Q = K_{eq}$, then the system is at EQUILIBRIUM and no shift will occur
If $Q < K_{eq}$, then $\frac{[PRODUCTS]}{[REACTANTS]}$ is **TOO SMALL** and shift right, more PRODUCTS
If $Q > K_{eq}$, then $\frac{[PRODUCTS]}{[REACTANTS]}$ is **TOO BIG** and shift left, more REACTANTS

7. Determining the direction of shift; Trial K_{eq}

$K_{eq} = 49$ for the equilibrium:

$$2NO(g) + O_2(g) \rightleftarrows 2NO_2(g)$$

If 2.0 mol of NO(g), 0.20 mol of O_2(g) and 0.40 mol of NO_2(g) are put into a 2.0 L bulb, which way will the reaction shift in order to reach equilibrium? Support your answer with the appropriate calculations.

$[NO] = \frac{2.0\text{mol}}{2.0L} = 1M$

$[O_2] = \frac{0.20\text{mol}}{2.0} = 0.10M$

$[NO_2] = \frac{0.40\text{mol}}{2.0L} = 0.20M$

$$Q = \frac{[NO_2]^2}{[NO]^2[O_2]}$$

$$Q = \frac{(0.20)^2}{(1.0)^2(.10)} = 0.4$$

$Q < K_{eq}$ ⇒ need top to get bigger

⇒ shift to products