ICE Tables

- If we place only reactants in a container, the system will reach an equilibrium
  - ✱ Therefore, we need to be able to calculate the *equilibrium* concentrations based on the *initial* concentrations
- ICE tables are a convenient way to organize and calculate the changes in the concentrations of products and reactants for a system that reaches equilibrium
  - "ICE" stands for the **i**nitial concentration, **c**hange in concentration, and **e**quilibrium concentration of all chemicals involved in a reaction system arrange into a table format
  - ✱ ICE table only contain *concentration* values

EXAMPLES:

1. Consider the reaction for the decomposition of hydrogen iodine at 448°C. The initial concentration of $HI_{(g)}$ was 1.00 mmol/L. Once an equilibrium was established, the concentration of $HI_{(g)}$ was measured to be 0.078 mmol/L. Calculate the equilibrium constant (K_c).

↳ need equilibrium concentrations ∴ ICE table!

	$2HI_{(g)}$ $\rightleftharpoons$	$H_{2(g)}$ +	$I_{2(g)}$
I	1.00	0	0
C	$-2x$	$+x$	$+x$
E	$1.00-2x$	x	x

b/c no products initally present

b/k being consumed

b/c being produced

Set table up with variables first!

✱ table set up in mmol/L ✱

$$K_c = \frac{[H_2][I_2]}{[HI]^2} = \frac{(x)(x)}{(1.00-2x)^2} = \frac{x^2}{(1.00-2x)^2}$$

but $[HI]_{equ.} = 1.00-2x = 0.078$

$$1.00 - 0.078 = 2x$$
$$0.922 = 2x$$
$$0.461 = x$$

$$K_c = \frac{(0.461)^2}{(0.078)^2} = 34.9311...$$

$$\boxed{K_c = 35}$$

2. Nitrogen dioxide can break down into nitrogen monoxide and oxygen. The equilibrium constant for this reaction is $Kc = 0.40$. If the equilibrium concentration of $NO_{2(g)}$ is 0.20 mol/L and the equilibrium concentration of $NO_{(g)}$ is 1.0 mol/L, what is the equilibrium concentration of $O_{2(g)}$? ↳ ∴ don't use ICE table !

$$2\,NO_2 \rightleftharpoons 2\,NO + O_2$$

$$\therefore \quad K_c = \frac{[O_2][NO]^2}{[NO_2]^2} \quad \Rightarrow \quad [O_2] = \frac{K_c\,[NO_2]^2}{[NO]^2}$$

$$[O_2] = \frac{(0.40)(0.20)^2}{(1.0)^2} = 0.016$$

$$\boxed{[O_2] = 0.016\,mol/L}$$

3. Ammonia gas ($NH_{3(g)}$) is produced in industrial amounts for use in the production of fertilizers. The most well-known industrial process to produce ammonia gas in large quantities is using the Haber-Bosch process as shown below.

$$N_{2(g)} + 3H_{2(g)} \leftrightarrow 2NH_{3(g)}$$

The equilibrium constant for the Haber-Bosch process is 0.469. If 20.0 mol of $N_{2(g)}$ and 75.0 mol of $H_{2(g)}$ are placed in a 5.00L reaction vessel and 33.0 mol of ammonia is present at equilibrium, what is the equilibrium concentration of hydrogen gas?

* ICE table needs to be set up with concentration values!

$C = \frac{n}{V}$ $\therefore$ $[N_2] = \frac{20.0\,mol}{5.0\,L} = 4.00\,mol/L$

$[H_2] = \frac{75.0\,mol}{5.0\,L} = 15.0\,mol/L$

	$N_{2(g)}$	+ $3H_{2(g)}$	$\rightleftharpoons$ $2NH_{3(g)}$
I	4.00	15.0	0
C	$-x$	$-3x$	$+2x$
E	$4.00-x$	$15.0-3x$	$2x$

from ICE table

but $[NH_3]_{equil.} = \frac{33.0\,mol}{5.0\,L} = 6.6\,mol/L = 2x$

$\therefore x = 3.3\,mol/L$

$[H_2]_{equil} = \underbrace{15.0 - 3x}_{\text{from ICE table}} = 15.0 - 3(3.3) = 5.1\,mol/L$

Note: we didn't even need the $K_c = 0.469$!

$\boxed{[H_2]_{equil.} = 5.1\,mol/L}$

***Now try pg. 658 #21, 23 & Practice Problems. More complex problem pg. 658 #22 ***

Practice Problems

1. Consider the equilibrium system:

$$CO_{(g)} + H_2O_{(g)} \leftrightarrow CO_{2(g)} + H_{2(g)}$$

Initially, 0.75 mol of water and 0.60 mol of carbon monoxide are placed in a 3.0L reaction vessel. At equilibrium, 0.30 mol of carbon dioxide is present. Calculate the equilibrium constant for the system. **[0.67]**

2. Consider the equilibrium system:

$$H_{2(g)} + Br_{2(g)} \leftrightarrow 2HBr_{(g)}$$

Initially, 0.25 mol of hydrogen and 0.25 mol of bromine are place in a 500mL reaction vessel. The equilibrium constant for the reaction is 50. Calculate the equilibrium concentration of bromine when the equilibrium concentration of hydrogen bromide is 0.78mol/L. **[0.11mol/L]**

3. Consider the equilibrium system:

$$2\ NO_{(g)} + Cl_{2(g)} \leftrightarrow 2\ NOCl_{(g)}$$

Initially, 5.0 mol of $NO_{(g)}$ and 5.0 mol of $Cl_{2(g)}$ were added to a 2.0 L container. As a result of the reaction, the equilibrium concentration of $NOCl_{(g)}$ became 0.96 mol/L. Determine the value of the equilibrium constant (K_c) for this reaction. **[0.19]**

End of Practice Problems

4. Nitrogen oxides from exhaust gases are a serious pollution problem. An environmental chemist is studying the following equilibrium reaction:

$$N_{2(g)} + O_{2(g)} \leftrightarrow 2NO_{(g)}$$

At a temperature of the exhaust gases from a particular engine, the value of K_c is 4.2×10^{-8}. The chemist puts 0.17 mol of nitrogen and 0.076 mol of oxygen in a rigid 2.0L cylinder. What is the concentration of nitrogen monoxide in the mixture at equilibrium?

← inital amounts ∴ use ICE table!

* first need concentration values!

$$C = \frac{n}{V} \quad \therefore \quad C_{N_2} = \frac{0.17\,mol}{2.0\,L} = 0.085\,mol/L$$

$$C_{O_2} = \frac{0.076\,mol}{2.0\,L} = 0.038\,mol/L$$

	$N_{2(g)}$	+ $O_{2(g)}$	$\rightleftharpoons 2NO_{(g)}$
I	0.085	0.038	0
C	0.085 − x	0.038 − x	+ 2x
E	0.085 − x	0.038 − x	2x

$$K_c = \frac{[NO]^2}{[N_2][O_2]} = \frac{(2x)^2}{(0.085-x)(0.038-x)}$$

"Foiled" / expanded

$$4.2 \times 10^{-8} = \frac{4x^2}{0.00323 - 0.123x + x^2}$$

a quadratic equation!

- Some equilibrium calculations can become very complex and time consuming to solve
- The previous example resulted in a quadratic equation which can be solved using the quadratic equation or by graphing
- However, for this example and ones that are more complex than a quadratic equation, we can use the **approximation rule**
- * The **approximation rule** states that if K_c x 1000 is less than the initial concentration of all reactants, then we can assume that the initial concentration of the reactants is the equilibrium concentration as well because K_c is so small which means hardly any reactants are being consumed
- Now let's finish our last example...

- first check to see if the approximation rule can apply

$4.2\times10^{-8} \times 1000 = 4.2\times10^{-5} < 0.085\ mol/L$ &
$0.038\ mol/L$

$\therefore$ use approximation rule!

$$4.2\times10^{-8} = \frac{4x^2}{(0.085-x)(0.038-x)}$$

can assume
$0.085-x \simeq 0.085$
$0.038-x \simeq 0.038$

$$4.2\times10^{-8} = \frac{4x^2}{(0.085)(0.038)}$$

$$4.2\times10^{-8} = \frac{4x^2}{0.00323} \Rightarrow 1.3566\times10^{-10} = 4x^2$$

$$3.3915\times10^{-11} = x^2$$

$$5.8236...\times10^{-6} = x$$

$$[NO]_{equ.} = 2x = 2(5.8236...\times10^{-6}\ mol/L)$$

$$\boxed{[NO]_{equ.} = 1.2\times10^{-5}\ mol/L}$$

Now try pg. 658 #24 & pg. 660# 25-29