Chemistry 201

ICE analysis

NC State University

ICE analysis

ICE stands for Initial, Change and Equilibrium. We will use the reaction stoichiometry to determine how the pressures will change as the reaction proceeds. In the method we are using here we assume that the total pressure can also change.

We can begin with the simplest possible chemical reaction.

$$cis - stilbene \leftrightarrows \; trans - stilbene$$

If we begin with a concentration of c_o molar cis-stilbene,
Then we can construct a table:
I = Initial concentrations
C = Change in concentrations during the reaction
E = Equilibrium concentrations

ICE analysis

The table for the isomerization of stilbene is:

	cis	trans
Initial	C_o	0
Change	-x	x
Equilibrium	$C_o - x$	x

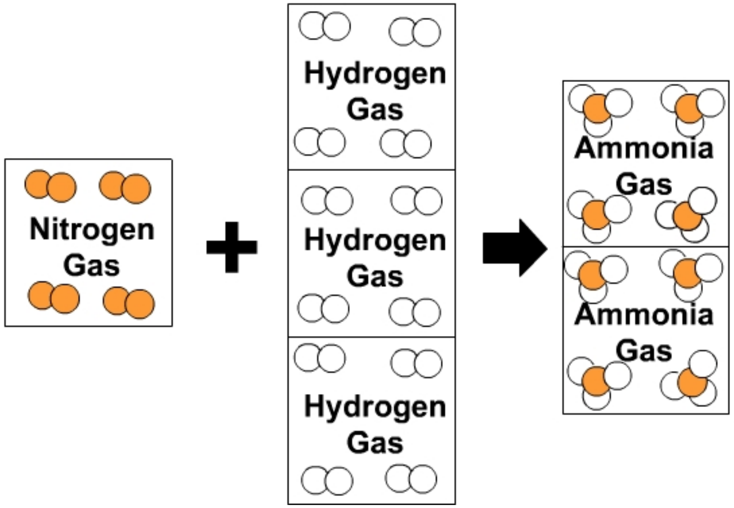
Then we substitute the equilibrium values into the equilibrium constant.

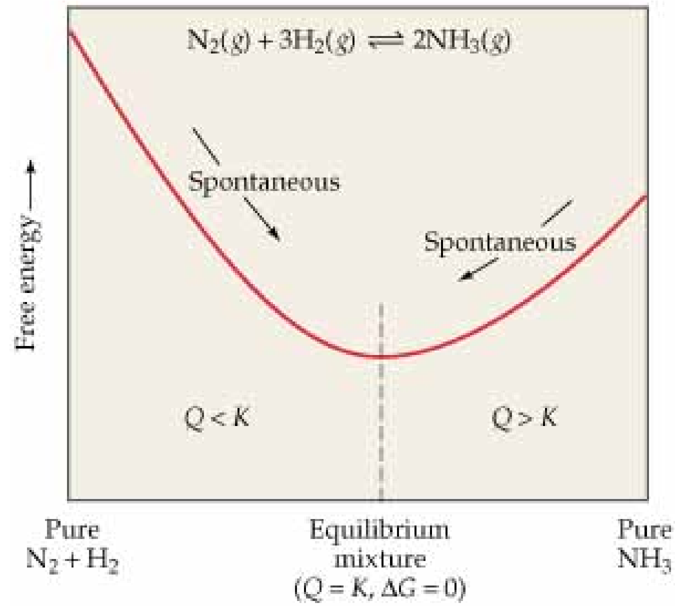
$$K = \frac{[trans]}{[cis]} = \frac{[x]}{[C_o - x]}$$

Therefore, in this case

$$x = \frac{C_o}{K+1}$$

ICE analysis for Haber-Bosch





The Haber-Bosch process is:

$$\frac{1}{2}N_2(g) + \frac{3}{2}H_2(g) \leftrightarrow NH_3(g)$$

We usually will have 0.8 atm of N_2 because that is the atmospheric value. If we add 2.4 atm of H_2 then we have a stoichiometric ratio to start with. Then we can construct an ICE table.

Construct a ICE table showing Initial, Change and Equilibrium pressures (or concentrations)

Using the initial pressures and the stoichiometry we can Determine the equilibrium pressures in terms of a reaction Progress variable, x. This is shown in the table.

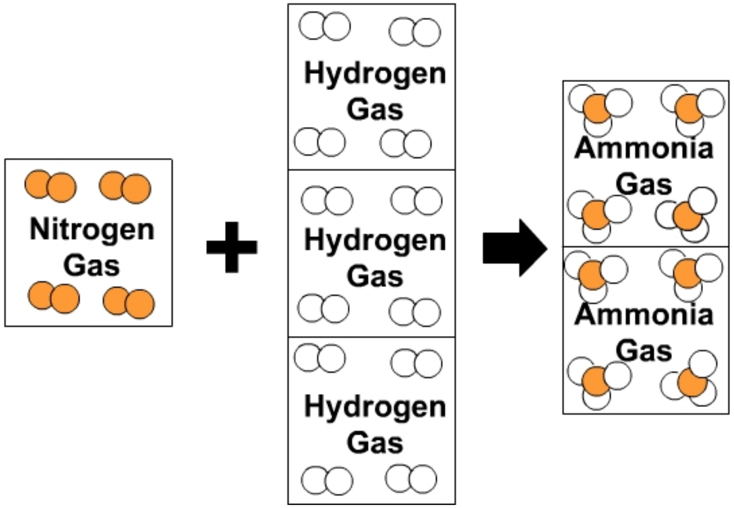
ICE	N_2	H_2	NH_3
Initial	0.8	2.4	0
Change	-0.5x	-1.5x	x
Equil.	0.8-0.5x	2.4-1.5x	x

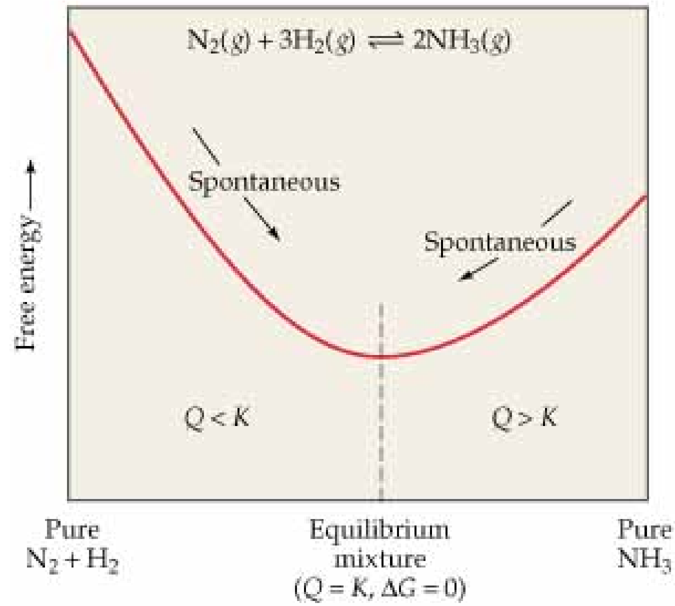
Thus, at equilibrium the pressures should be:

$$P_{N_2} = 0.8 - 0.5x \text{ atm} \ ; \ P_{H_2} = 2.4 - 1.5x \text{ atm} \ ; \ P_{NH_3} = x$$

These values are then substituted into the equilibrium constant.

ICE analysis





Based on the stoichiometry for:

$$\frac{1}{2}N_2(g) + \frac{3}{2}H_2(g) \leftrightarrow NH_3(g)$$

We see that the equilibrium values can be determined by Solving the equation:

$$K = \frac{x}{(0.8 - 0.5x)^{\frac{1}{2}}(2.4 - 1.5x)^{\frac{3}{2}}}$$

Solve for the reaction progress variable

We will solve a general form valid for any K.

$$K = \frac{x}{(0.8 - 0.5x)^{\frac{1}{2}}(2.4 - 1.5x)^{\frac{3}{2}}}$$

$$K = \frac{1}{3^{3/2}} \frac{x}{(0.8 - 0.5x)^2}$$

$$K(0.8 - 0.5x)^2 = \frac{x}{3^{3/2}}$$

$$K(0.64 - 0.8x + 0.25x^2) = \frac{x}{3^{3/2}}$$

$$0.64 - \left(0.8 + \frac{0.192}{K}\right)x + 0.25x^2 = 0$$

$$x = \frac{\left(0.8 + \frac{0.192}{K}\right) \pm \sqrt{\left(0.8 + \frac{0.192}{K}\right)^2 - 0.64}}{0.5}$$

What are the equilibrium pressures when K = 1

K is temperature dependent, so it can have different values. Just to test our solution, let's suppose that K = 1. This means that $\Delta G^o = 0$ for the reaction. It also means that the reaction should have equal molar ratios of reactants and products weighted the stoichiometry, of course.

$$x = \frac{0.992 \pm \sqrt{0.992^2 - 0.64}}{0.5} \qquad x = \frac{0.992 \pm 0.5865}{0.5}$$

$$x = 3.2 \text{ or } 0.8$$

Only the answer x = 0.8 makes physical sense.

$$P_{N_2} = 0.4\ \text{atm}\ ;\ P_{H_2} = 1.2\ \text{atm}\ ;\ P_{NH_3} = 0.8\ \text{atm}$$

Indeed, the pressures have the appropriate molar ratios.

Return to the smog reaction

Consider the reaction: $N_2O_4(g) \rightarrow 2\ NO_2(g)$

If the initial pressure of N_2O_4 is 1 atm (and NO_2 is 0 atm) calculate the pressure of both species at equilibrium (assuming the total pressure can change).

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If the initial pressure of N_2O_4 is 1 atm (and NO_2 is 0 atm) calculate the pressure of both species at equilibrium (assuming the total pressure can change).

We create an ICE table using the stoichiometry.

ICE	N_2O_4	NO_2
Initial	1.0	0.0
Change	-x	+2x
Equil.	1 - x	2x

Consider the reaction: $N_2O_4(g) \rightarrow 2\ NO_2(g)$

If the initial pressure of N_2O_4 is 1 atm (and NO_2 is 0 atm) calculate the pressure of both species at equilibrium.

We can also write the result of the ICE analysis:

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

$$1-x \qquad\qquad 2x$$

Next, plug those expressions into the equilibrium Constant:

$$K = \frac{{P_{NO_2}}^2}{P_{N_2O_4}}$$

$$K = \frac{(2x)^2}{(1-x)}$$

After plugging the values into the equlibrium constant formula,

$$K = \frac{(2x)^2}{(1-x)}$$

we solve for the unknown, x

$$K - Kx - 4x^2 = 0$$

Noting that K = 0.11 (as determined previously)

$$x = -\frac{K \pm \sqrt{K^2 + 16K}}{8}$$

and

$$x = 0.152$$