

ICE Chart Calculations

1. What is an ICE chart?

An ICE chart is a means of organizing data when solving a problem for an equilibrium reaction. The key for understanding problem solving is: Stoichiometry is used for reactions that are said to run to completion or when trying to determine theoretical results.

ICE charts are used for any and all equilibrium processes.

The basic format of an ICE chart is:

| | | | | | | | | | |
|----------|--------------|---|--------------|----------------------|--------------|---|--------------|---|------------|
| | $aA_{(aq)}$ | + | $bB_{(aq)}$ | \rightleftharpoons | $cC_{(aq)}$ | + | $dD_{(aq)}$ | + | $eE_{(s)}$ |
| <i>I</i> | $[A]_i$ | | $[B]_i$ | | $[C]_i$ | | $[D]_i$ | | — |
| <i>C</i> | $-ax$ | | $-bx$ | | $+cx$ | | $+dx$ | | — |
| <i>E</i> | $[A]_i - ax$ | | $[B]_i - bx$ | | $[C]_i + cx$ | | $[D]_i + dx$ | | — |

$[]_i$: initial concentration of each species

$-a, -b$: are the molar coefficients from the balanced equation.
The negative sign reflects that the reactants are used up as the reaction proceeds in the forward direction.

$+c, +d$: are the molar coefficients from the balanced equation.
The positive sign reflects that the products are produced as the reaction proceeds in the forward direction.

x : reflects the amount of product formed and reactant used per mole.

The signs would be reversed if the reaction proceeded in the reverse direction.

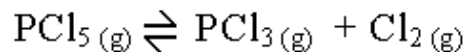
E is not included in the chart because it is a solid. Remember solids and liquids do not affect equilibrium – therefore they are not included in equilibrium calculations.

It is also important to note that concentration of the various species is plugged in, not moles! If you are dealing with a gaseous solution, concentration can be replaced with partial pressure data.

This chart is useful because it indicates the values at equilibrium of all species in the reaction. As we have already discussed, equilibrium values, plugged into the appropriate equation yields K. Thus we can use these values to solve for K or, if given K, we can determine equilibrium

concentrations.

2. Consider:



$$K_p = \frac{(P_{\text{PCl}_3}) (P_{\text{PCl}_3})}{(P_{\text{Cl}_2})}$$

As a first step to solving these types of problems it is a good idea to get the equilibrium expression, as it will be used in the solving process 95% of the time.

If an evacuated flask is filled with 0.50 atm of pure PCl_5 what is K_p if there is a pressure of 0.84 atm after equilibrium has been achieved?

| | $\text{PCl}_5(\text{g})$ | \rightleftharpoons | $\text{PCl}_3(\text{g})$ | + | $\text{Cl}_2(\text{g})$ |
|----------|--------------------------|----------------------|--------------------------|---|-------------------------|
| <i>I</i> | 0.50 atm | | 0 | | 0 |
| <i>C</i> | -x | | +x | | +x |
| <i>E</i> | 0.50 - x | | x | | x |

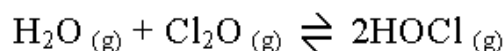
$$\frac{(0.50 - x)}{P_{\text{PCl}_5}} + \frac{(x)}{P_{\text{PCl}_3}} + \frac{(x)}{P_{\text{Cl}_2}} = \frac{0.84 \text{ atm}}{P_{\text{total}}}$$

@ equilibrium

$$x = 0.34 \text{ atm}$$

$$K_p = \frac{(P_{\text{PCl}_3}) (P_{\text{PCl}_3})}{(P_{\text{Cl}_2})} = \frac{(x) (x)}{(0.50 - x)} = \frac{(0.34 \text{ atm}) (0.34 \text{ atm})}{(0.16 \text{ atm})} = \boxed{0.72}$$

3. At 25°C, $K=0.090$ for:



$$K = \frac{[\text{HOCl}]^2}{[\text{H}_2\text{O}] [\text{Cl}_2\text{O}]}$$

Calculate the equilibrium concentrations of all species if 1.5g H₂O and 2.3g Cl₂O are mixed in a 1.4L flask.

$$[\text{H}_2\text{O}] = 1.5\text{g H}_2\text{O} \frac{1\text{ mol H}_2\text{O}}{18.02\text{g H}_2\text{O}} \frac{1}{1.4\text{L of sol'n}} = 0.0595\text{M H}_2\text{O}$$

$$[\text{Cl}_2\text{O}] = 2.3\text{g Cl}_2\text{O} \frac{1\text{ mol Cl}_2\text{O}}{86.90\text{g Cl}_2\text{O}} \frac{1}{1.4\text{L of sol'n}} = 0.0189\text{M Cl}_2\text{O}$$

| | H ₂ O _(g) | + Cl ₂ O _(g) | ⇌ | 2HOCl _(g) |
|----------|---------------------------------|------------------------------------|---|----------------------|
| <i>I</i> | 0.0595 M | 0.0189 M | | 0 |
| <i>C</i> | -x | -x | | +2x |
| <i>E</i> | 0.0595 - x | 0.0189 - x | | 2x |

$$K = \frac{[\text{HOCl}]^2}{[\text{H}_2\text{O}] [\text{Cl}_2\text{O}]} = \frac{(2x)^2}{(0.0595 - x)(0.0189 - x)} = 0.090$$

$$\frac{3.91x^2}{a} + \frac{7.06 \times 10^{-3} x}{b} - \frac{1.02 \times 10^{-4}}{c} = 0$$

This is a more complicated problem – x cannot be determined by simple factoring processes. The quadratic equation will have to be used to solve for x.

Use the quadratic to solve for x

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

The corresponding coefficients need to be plugged into the quadratic to solve for x. There will be two possible solutions for x – only one of them will work as a solution to the problem.

$$x = 4.29 \times 10^{-3} \text{ or } x = -0.0931 \leftarrow$$

(a negative answer doesn't make sense)

Now plug your value for x into the equilibrium expression from the ICE chart to get the final answers.

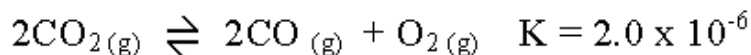
$$[H_2O] = 0.0595 - 4.29 \times 10^{-3} = 0.0552 \text{ M}$$

$$[Cl_2O] = 0.0189 - 4.29 \times 10^{-3} = 0.0146 \text{ M}$$

$$[HOCl] = 2(4.29 \times 10^{-3}) = 8.58 \times 10^{-3} = 8.58 \times 10^{-3} \text{ M}$$

These problems are the most tedious to solve. There is a lot of room for algebraic error along the way. For many problems there is a simplification that can be made that allows one to bypass the quadratic. The proceeding problem illustrates this method.

4. Consider :



$$K = \frac{[CO]^2 [O_2]}{[CO_2]^2}$$

If 2.0 mol CO₂ is initially placed into a 3.5L vessel, calculate equilibrium concentrations of all species.

$$[CO_2] = \frac{2.0 \text{ mol}}{3.5 \text{ L}} = 0.57 \text{ M}$$

| | | | | | |
|----------|--------------------------|----------------------|------------------------|---|------------------------|
| | $2\text{CO}_2(\text{g})$ | \rightleftharpoons | $2\text{CO}(\text{g})$ | + | $\text{O}_2(\text{g})$ |
| <i>I</i> | 0.57 M | | 0 | | 0 |
| <i>C</i> | $-2x$ | | $+2x$ | | $+x$ |
| <i>E</i> | $0.57 - 2x$ | | $2x$ | | x |

$$K = \frac{[\text{CO}]^2 [\text{O}_2]}{[\text{CO}_2]^2} = \frac{(2x)^2 (x)}{(0.57 - 2x)^2} = 2.0 \times 10^{-6}$$

Now at this point solving could get VERY complicated, we would be dealing with a cubic – that is unless we make an assumption.

Do you remember what the value of K indicates about reaction/equilibrium point? A $K < 1$ indicates that a reaction does not proceed very much toward the products. In this question $K = 2.0 \times 10^{-6}$, this is a VERY small K – meaning a relatively negligible amount of the reactant is used up. Practically, this means we are assuming...

$$0.57 - 2x = 0.57$$

To understand this a little bit better consider

$$1000 - 0.00001 = 999.99999$$

If you take significant figure rules into account this number is as good as 1000. Though there is a tiny amount subtracted... it is not significant enough to warrant concern.

This begs the question, at what point is a number significant enough to warrant concern? If the value of x is greater than 5% of the initial amount than this assumption cannot be made.

Let's see all of this information in practice...

$$\frac{(2x)^2 (x)}{(0.57)^2} = 2.0 \times 10^{-6}$$

$$x = 5.46 \times 10^{-3} M$$

$$\frac{\text{change}}{\text{initial concentration}} = \frac{2x}{0.57} = \frac{2(5.46 \times 10^{-3})}{0.57} \times 100 = 1.92\%$$

Smaller than 5%, so the assumption is valid.

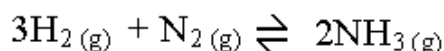
Thus answers can be reported as:

$$[CO_2] = 0.57 - 2(5.46 \times 10^{-3}) = \boxed{0.56 M}$$

$$[CO] = 2(5.46 \times 10^{-3}) = \boxed{0.0109 M}$$

$$[O_2] = \boxed{5.46 \times 10^{-3} M}$$

5. Consider



As per the usual steps – I write down the expression for K first.

$$K = \frac{[NH_3]^2}{[H_2]^3 [N_2]}$$

If at equilibrium, the concentrations for H₂, N₂ and NH₃ are 5.0M, 8.0M, and 4.0M, respectively. What were the initial concentrations of H₂ and N₂ put into the container?

I then proceed to getting all of the data, form the question, organized in an ICE chart.

| | 3H ₂ (g) | + N ₂ (g) | ⇌ | 2NH ₃ (g) |
|----------|---------------------|----------------------|---|----------------------|
| <i>I</i> | <i>A</i> | <i>B</i> | | <i>0</i> |
| <i>C</i> | - 3 <i>x</i> | - <i>x</i> | | +2 <i>x</i> |
| <i>E</i> | 5.0M | 8.0M | | 4.0M |

So now, looking at the question and the information. The question asks for the initial values of H_2 and N_2 . I have 3 unknowns – A, B and x. What would the logical next step be? Do I need to use K? Could it help me solve for initial, non-equilibrium concentrations? No, not really.

Maybe you notice that only x stands in the way of your solving for A and B.

$$\begin{aligned}A - 3x &= 5.0M \\ \text{and} \\ B - x &= 8.0M\end{aligned}$$

How can we solve for x?

Look at the information for NH_3 .

$$\begin{aligned}2x &= 4.0M \\ x &= 2.0M\end{aligned}$$

Now it's just a matter of plugging in the value of x.

$$\begin{aligned}[H_2] &= (A - 3x) = 5.0M \quad (A - 3(2.0M)) = 5.0M \quad A = \boxed{11.0M} \\ [N_2] &= (B - x) = 8.0M \quad (B - 2.0M) = 8.0M \quad B = \boxed{10.0M}\end{aligned}$$

As was previously stated, K will be used 95% of the time... so there are occasions where it is unnecessary. It never hurts to jot it down though – especially if you tend to like to follow a systematic method for solving. You'll just need to remember to be flexible.