Calculate Equilibrium Concentrations from Initial Conditions

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Calculating K_c from a known set of equilibrium concentrations seems pretty clear. You just plug into the equilibrium expression and solve for K_c.

Calculating equilibrium concentrations from a set of initial conditions takes more calculation steps. In this type of problem, the K_c value will be given

The best way to explain is by example. Just in case you are not sure, the subscripted zero, as in $[H_2]_o$, means the initial concentration.

Example #1: Given this equation:

$$H_2 + I_2 \rightleftharpoons 2\ HI$$

Calculate all three equilibrium concentrations when $[H_2]_o = [I_2]_o = 0.200$ M and $K_c = 64.0$.

Solution:

1) The solution technique involves the use of what is most often called an ICEbox. Here is an empty one:

	$[H_2]$	$[I_2]$	$[HI]$
Initial			
Change			
Equilibrium			

The ChemTeam hopes you notice that I, C, E are the first initials of Initial, Change, and Equilibrium.

2) Now, let's fill in the initial row. This should be pretty easy:

	$[H_2]$	$[I_2]$	[HI]
Initial	0.200	0.200	0
Change			
Equilibrium			

The first two values were specified in the problem and the last value ([HI] = 0) come from the fact that the reaction has not yet started, so no HI could have been produced yet.

3) Now for the change row. This is the one that causes the most difficulty in understanding:

	$[H_2]$	$[I_2]$	[HI]
Initial	0.200	0.200	0
Change	- x	- x	+ 2x
Equilibrium			

The minus sign comes from the fact that the H_2 and I_2 amounts are going to go down as the reaction proceeds.

x signifies that we know some H_2 and I_2 get used up, but we don't know how much. What we do know is that an EQUAL amount of each will be used up. We know this from the coefficients of the equation. For every one H_2 used up, one I_2 is used up also.

The positive signifies that more HI is being made as the reaction proceeds on its way to equilibrium.

The two is important. HI is being made twice as fast as either H_2 or I_2 are being used up.

In fact, always use the coefficients of the balanced equation as coefficients on the "x" terms.

In problems such as this one, never use more than one unknown. Since we have only one equation (the equilibrium expression) we cannot have two unknowns.

4) The equilibrium row should be easy. It is simply the initial conditions with the change applied to it:

	$[H_2]$	$[I_2]$	[HI]
Initial	0.200	0.200	0
Change	- x	- x	+ 2x
Equilibrium	0.200 - x	0.200 - x	2x

5) We are now ready to put values into the equilibrium expression. For convenience, here is the equation again:

$H_2 + I_2 \rightleftharpoons 2\ HI$

and the equilibrium expression is:

$K_c = [HI]^2 / ([H_2]\ [I_2])$

6) Plugging values into the expression gives:

$64.0 = (2x)^2 / ((0.200 - x)\ (0.200 - x))$

Two points need to be made before going on:

1) Where did the 64.0 value come from? It was given in the problem.
2) Make sure to write $(2x)^2$ and not $2x^2$. As you well know, they are different. This mistake happens a LOT!!

6) Both sides are perfect squares (done so on purpose), so we square

root both sides to get:

$$8.00 = (2x) / (0.200 - x)$$

From there, the solution should be easy and results in x = 0.160 M.

7) This is not the end of the solution since the question asked for the equilibrium concentrations, so:

$[H_2] = 0.200 - 0.160 = 0.040$ M
$[I_2] = 0.200 - 0.160 = 0.040$ M
$[HI] = 2\ (0.160) = 0.320$ M

8) You can check for correctness by plugging back into the equilibrium expression:

$$x = (0.320)^2 / ((0.040)\ (0.040))$$

Since x = 64.0. we know that the problem was correctly solved.

In the second example, the quadratic formula will be used.

Example #2: Given this equation:

$$PCl_3 + Cl_2 \rightleftharpoons PCl_5$$

Calculate all three equilibrium concentrations when $K_c = 16.0$ and $[PCl_5]_o = 1.00$ M.

Solution:

1) Here is the completed ICEbox:

	$[PCl_3]$	$[Cl_2]$	$[PCl_5]$
Initial	0	0	1.00
Change	+ x	+ x	- x
Equilibrium	x	x	1.00 - x

2) The equilibrium expression is:

$K_c = [PCl_5] / ([PCl_3] [Cl_2])$

Substituting gives:

$16.0 = (1.00 - x) / (x \text{ times } x)$

3) After suitable manipulation (which you can perform yourself), we arrive at this quadratic equation in standard form:

$16x^2 + x - 1 = 0$

4) Using the quadratic formula, which is $x = (- b \pm \text{square root}[b^2 - 4ac]) / 2a$, we obtain:

$x = (- 1 + \text{square root}[1^2 - (4) (16) (-1)]) / 32$

After suitable calculations, we find x = 0.221.

Please notice that the negative root was dropped, because negative b turned out to be negative one. The answer obtained in this type of problem CANNOT be negative.

Why?

Because we are dealing with the amount of a physical substance in mol / L. Amounts of substances are always represented with positive numbers. An amount of a substance with physical reality cannot be represented with negative numbers.

5) Determination of the equilibrium amounts and checking for correctness by inserting back into the equilibrium expression is left to the student.

The third example will be one in which both roots give positive answers. The question then becomes how to determine which root is the correct one to use.

Example #3: Given this equation:

$$COCl_2 \rightleftharpoons CO + Cl_2$$

Calculate all three equilibrium concentrations when $K_c = 0.680$ with $[CO]_o = 0.500$ and $[Cl_2]_o = 1.00$ M.

Solution:

1) Here is the completed ICEbox:

	$[COCl_2]$	[CO]	$[Cl_2]$
Initial	0	0.500	1.00
Change	+ x	- x	- x
Equilibrium	x	0.500 - x	1.00 - x

2) The equilibrium expression is:

$$K_c = ([CO]\,[Cl_2]) / [COCl_2]$$

Substituting into the expression gives:

$$0.680 = ((0.5 - x)\,(1 - x)) / x$$

3) After some manipulation (left to the student), we arrive at this quadratic equation, in standard form:

$$x^2 - 2.18x + 0.5 = 0$$

4) Using the quadratic formula, we have this:

$x = (2.18 \pm \text{square root}[(2.18)^2 - (4) (1) (0.5)]) / 2$

After some manipulation (left to the student), we arrive at:

$(2.18 \pm 1.66) / 2$

5) Both roots yield positive values, so how do we pick the correct one?

The answer lies in the fact that x is not the final answer, whereas (0.5 - x) is. It is the term (0.5 - x) which must be positive.

So the root of 1.92 is rejected in favor of the 0.26 value and the day is saved!!

[Let's do some more]

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