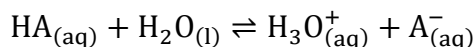


Scenario 1 – Approximation Rule

One of the best examples of the use of the quadratic equation in equilibrium is solving for the hydrogen ion concentration of a weak acid solution.

Weak acids do not ionize fully - there is an equilibrium. The general equation looks as such:



(where HA is a term for a monoprotic acid)

Example: What is the $\text{H}_3\text{O}_{(\text{aq})}^+$ of 0.1 mol/L $\text{CH}_3\text{COOH}_{(\text{aq})}$ (acetic acid) given $K_a = 1.8 \times 10^{-5}$?

Write out the equation and make an ICE (Initial, Change, Equilibrium) Table:

	$\text{CH}_3\text{COOH}_{(\text{aq})}$	+	$\text{H}_2\text{O}_{(\text{l})}$	\rightleftharpoons	$\text{H}_3\text{O}_{(\text{aq})}^+$	+	$\text{CH}_3\text{COO}_{(\text{aq})}^-$
	Acid		Base		Conjugate Acid		Conjugate Base
Initial	0.1				~0		0
Change	-x				+x		+x
Equilibrium	0.1-x				x		x

*I write ~0 as the initial concentration for $\text{H}_3\text{O}_{(\text{aq})}^+$ is 10^{-7} M and this is insignificant.

$$K_a = \frac{\text{products}}{\text{reactants}} = \frac{[\text{H}_3\text{O}_{(\text{aq})}^+][\text{CH}_3\text{COO}_{(\text{aq})}^-]}{[\text{CH}_3\text{COOH}_{(\text{aq})}]} = \frac{x^2}{0.1 - x}, K_a = 1.8 \times 10^{-5}$$

$$1.8 \times 10^{-5} = \frac{x^2}{0.1 - x}$$

Normally we would isolate for x and find that our equation looks like this:

$$x^2 + 1.8 \times 10^{-5}x - 1.8 \times 10^{-6} = 0$$

Which we then solve by using the quadratic equation:

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}, \text{ where } ax^2 + bx + c = 0$$

However, consider that if K is small and K equals products over reactants, then we have very few products.

This means x is tiny. Tiny enough to be insignificant – we can apply an approximation:

$$\text{If } \frac{[\text{initial concentration, I}]}{K_a} > 1000 \text{ then } [I - x] \cong [I]$$

$$\frac{0.1}{1.8 \times 10^{-5}} > 1000,$$

We introduce error in the 3rd significant figure or beyond by approximating our equation (green):

$$1.8 \times 10^{-5} = \frac{x^2}{0.1}$$

$$1.8 \times 10^{-6} = x^2, x = 0.001342 = [\text{H}_3\text{O}_{(\text{aq})}^+] = [\text{CH}_3\text{COO}_{(\text{aq})}^-]$$

Let's do another example:

Scenario 2 – Quadratic

Example: What is the H_3O^+ of 0.1 mol/L $\text{HOCCOOH}_{(\text{aq})}$ given $K_a = 5.6 \times 10^{-2}$?

	$\text{HOCCOOH}_{(\text{aq})}$	+	$\text{H}_2\text{O}_{(\text{l})}$	\rightleftharpoons	$\text{H}_3\text{O}^+_{(\text{aq})}$	+	$\text{HOCCOO}^-_{(\text{aq})}$
	Acid		Base		Conjugate Acid		Conjugate Base
Initial	0.1				~0		0
Change	-x				+x		+x
Equilibrium	0.1-x				x		x

$$K_a = \frac{\text{products}}{\text{reactants}} = \frac{[\text{H}_3\text{O}^+_{(\text{aq})}][\text{HOCCOO}^-_{(\text{aq})}]}{[\text{HOCCOOH}_{(\text{aq})}]} = \frac{x^2}{0.1 - x}, K_a = 5.6 \times 10^{-2}$$

$$\frac{0.1}{5.6 \times 10^{-2}} \gg 1000$$

Apparently, it is a bad idea to approximate in this case. Let's see why:

Quadratic

$$5.6 \times 10^{-2} = \frac{x^2}{0.1 - x}$$

$$x^2 + 5.6 \times 10^{-2}x - 5.6 \times 10^{-3} = 0$$

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}, \text{ where } ax^2 + bx + c = 0$$

$$x = \frac{-5.6 \times 10^{-2} \pm \sqrt{(5.6 \times 10^{-2})^2 - 4(1)(-5.6 \times 10^{-3})}}{2(1)}$$

$$x = \frac{-5.6 \times 10^{-2} \pm \sqrt{0.003136 + 0.0224}}{2}$$

$$x = \frac{-5.6 \times 10^{-2} \pm 0.15979987}{2}$$

$$x = -0.11 \text{ OR } 0.052$$

$$x = 0.052 = [\text{H}_3\text{O}^+_{(\text{aq})}] = [\text{CH}_3\text{COO}^-_{(\text{aq})}]$$

Approximation

$$5.6 \times 10^{-2} = \frac{x^2}{0.1}$$

$$5.6 \times 10^{-3} = x^2$$

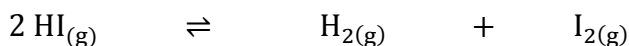
$$0.075 = x$$

In this case, the error is greater than ~ the third significant figure (this comes from our criteria of >1000 fold difference).

Notice also that the quadratic gives two answers – one that is real and another that is illogical (we cannot have a negative x as that would mean we shift to reactants with zero products)

Scenario 3 – Root of Both Sides

Hydrogen iodide gas is introduced into a container at 2.00 molar concentration. $\text{HI}_{(g)}$ then disintegrates into hydrogen gas and solid iodine. If the equilibrium constant is 10.0, what is the concentration of hydrogen gas in the container?



Initial	2.00		0	0
Change	-x		+x	+x
Equilibrium	2.00-x		x	x

We get

$$K = \frac{[\text{H}_{2(g)}][\text{I}_{2(g)}]}{[\text{HI}_{(g)}]^2} = \frac{[x][x]}{[2.00 - x]^2} = \frac{x^2}{(2.00 - x)^2} = 10.0$$

We can do the quadratic or we notice we can do the root of both sides:

$$\frac{x^2}{(2.00 - x)^2} = 10.0$$

$$\sqrt{\frac{x^2}{(2.00 - x)^2}} = \sqrt{10.0}$$

$$\frac{x}{2.00 - x} = 3.16$$

$$x = 6.32 - 3.16x$$

$$4.16x = 6.32, x = 1.52$$

Other Cases

If you are ever at the situation where you have a cubic (x^3), quartic (x^4), etc. equation to solve, this means you missed an opportunity to either do a root of both sides or an approximation. An example can be:

$$\frac{x^2}{(2 - x)^4} = 100$$

$$\sqrt{\frac{x^2}{(2 - x)^4}} = \sqrt{100}$$

$$\frac{x}{(2 - x)^2} = 10$$

This difficult example is followed by solving a quadratic.

Some difficult questions have an incredibly large or incredibly small x value and you must deduce that you approximate without referencing any kind of rule.

$$\frac{x}{(2-x)^4} = 5.6 \times 10^{-23}$$

$$\frac{x}{(2)^4} = 5.6 \times 10^{-23}$$

$$x = 8.96 \times 10^{-22}$$