Slide 1

Chemical Equilibrium

Some more complicated applications

Slide 2

The ICE chart is a powerful tool for many different equilibrium problems

But you can't always make a simplifying assumption, and that means that you may need to do a little algebra

Slide 3

A Quadratic Equation

A quadratic equation is a 2nd order polynomial of the general form:

$a x^2 + b x + c = 0$

Where a, b, and c represent number coefficients and x is the variable

Slide 4

The Quadratic Formula

$a x^2 + b x + c = 0$

All quadratic equations have a solution for x that is given by:

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

Slide 5

Equilibrium & the Quadratic Formula

If you cannot make a simplifying assumption, many times you will end up with a quadratic equation for an equilibrium constant expression.

You can end up with a 3rd, 4th, 5th, etc. order polynomial, but I will not hold you responsible for being able to solve those as there is no simple formula for the solution.

Slide 6

A sample problem.

A mixture of 0.00250 mol $H_{2\,(g)}$ and 0.00500 mol of $I_{2\,(g)}$ was placed in a 1.00 L stainless steel flask at 430 °C. The equilibrium constant, based on concentration, for the creation of HI from hydrogen and iodine is 54.3 at this temperature.

What are the equilibrium concentrations of all 3 species?

Slide 7

Determining the concentrations

ICE - ICE - BABY - ICE – ICE

The easiest way to solve this problem is by using an ICE chart.

We just need a BALANCED EQUATION

Slide 8

An ICE Chart

$H_{2\,(g)} + I_{2\,(g)} \leftrightarrow 2\ HI_{(g)}$

Slide 9

An ICE Chart

$H_{2\,(g)} + I_{2\,(g)} \leftrightarrow 2\ HI_{(g)}$

	H_2	I_2	HI
I	0.00250 M	0.00500 M	0 M
C	-x	-x	+2x
E	0.00250 – x	0.00500 – x	2x

Slide 10

Plug these numbers into the equilibrium constant expression.

$$K_c = 54.3 = \frac{[HI]^2}{[H_2][I_2]}$$

$$K_c = 54.3 = \frac{[2x]^2}{[0.00250 - x][0.00500 - x]}$$

I could start by assuming x<<0.00250, it is always worth taking a look at the "easy" solution.

Slide 11

Assuming x is small…

$$K_c = 54.3 = \frac{[2x]^2}{[0.00250 - x][0.00500 - x]}$$

IF x<<0.00250

$$K_c = 54.3 = \frac{[2x]^2}{[0.00250][0.00500]}$$

$6.788 \times 10^{-4} = 4x^2$

$1.697 \times 10^{-4} = x^2$

$0.0130 = x$

THE ASSUMPTION DOES NOT WORK!

Slide 12

We're going to have to use the quadratic formula

$$K_c = 54.3 = \frac{[2x]^2}{[0.00250 - x][0.00500 - x]}$$

$$54.3 = \frac{[2x]^2}{[x^2 - 0.00750x + 1.25 \times 10^{-5}]}$$

$54.3(x^2 - 0.00750\ x + 1.25 \times 10^{-5}) = 4x^2$

$54.3x^2 - 0.407\ x + 6.788 \times 10^{-4} = 4x^2$

$50.3x^2 - 0.407\ x + 6.788 \times 10^{-4} = 0$

On to the Quadratic Formula

Slide 13

Using the quadratic formula

$50.3x^2 - 0.407x + 6.788\times10^{-4} = 0$

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

$$x = \frac{-(-0.407) \pm \sqrt{(-0.407)^2 - 4(50.3)(6.78 \times 10^{-4})}}{2(50.3)}$$

$$x = \frac{0.407 \pm \sqrt{0.1656 - 0.1366}}{100.6}$$

$$x = \frac{0.407 \pm \sqrt{0.170}}{100.6}$$

X = 0.005736 OR 0.002356

Slide 14

There are 2 roots…

All 2nd order polynomials have 2 roots, BUT only one will make sense in the equilibrium problem

x = 0.005736 OR 0.002356

Which is correct?

Look at the ICE chart and it will be clear.

Slide 15

x = 0.005736 OR 0.002356

$H_{2\,(g)} + I_{2\,(g)} \leftrightarrow 2\,HI_{(g)}$

	H_2	I_2	HI
I	0.00250 M	0.00500 M	0 M
C	-x	-x	+2x
E	0.00250 – x	0.00500 – x	2x

If x = 0.005736, then the equilibrium concentrations of the reactants would be NEGATIVE! This is a physical impossibility.

Slide 16

SO x = 0.002356

$$H_{2\,(g)} + I_{2\,(g)} \leftrightarrow 2\,HI_{(g)}$$

	H_2	I_2	HI
I	0.00250 M	0.00500 M	0 M
C	-0.002356	-0.002356	+2(0.002356)
E	0.000144 M	0.002644 M	0.00471 M

And you are done!

Slide 17

X IS NOT THE ANSWER

X IS A WAY TO GET TO THE ANSWER