Solution Calculations - Two Examples

The conversion between solution units is a mechanical exercise. What I mean by that is that once one executes and sees how these units are changed, then it becomes a simple exercise that requires little effort. The bad news? You have to go through it and practice. However, just like driving a car, it becomes second nature after a while.

Below are two examples with explanation. If one has two pieces of information, then most all other items can be found in most cases.

NOTE! Look for %m/m or molality! As we will see in the following examples, if one has one of these, then one has most everything. Let's begin.

Example 1: Consider a 0.25 molar solution of glucose (MW = 180) having a density of 0.915 g/ml.

Calculate % m/v, % m/m, ppt m/m, ppm m/v, molality and mole fraction.

Step 1: Write and define what you have.

 $0.25 \cdot M = \frac{0.250 \text{ moles_glucose}}{L_{\text{solution}}} = \frac{0.250 \cdot \text{mole_glucose}}{1000 \cdot \text{mL_solution}}$

Note: Notice how I am very specific as to grams of what and mL of what. Do this! It's a pain, but will reap benefits.

Step 2: Although there are many approaches that are effective, I personally elect to convert from M to % m/v. It's the easiest in my opinion. to wit...

 $\frac{0.250 \cdot \text{mole}_\text{glucose}}{1000 \cdot \text{mL}_\text{solution}} = \frac{0.0250 \cdot \text{mols}_\text{glucose}}{100 \cdot \text{mL}_\text{solution}}$

Note: A simple division by 10 and the denominator is right where I want it! Note, convert the numerator to grams and Viola!

$$\frac{0.0250 \cdot \text{mols_glucose}}{100 \cdot \text{mL_solution}} \cdot \left(\frac{180 \cdot \text{g_glucose}}{\text{moles_glucose}}\right) = \frac{4.50 \cdot \text{g_glucose}}{100 \cdot \text{mL_glucose}} = 4.50\% \text{ m/v}$$

Notice how I kept the denominator at 100 mL as required by the definition.

Handy note!! The conversion from %m/v to % m/m or back is accomplished using the density!

 $\frac{4.50 \cdot \text{g}_{\text{glucose}}}{100 \cdot \text{mL}_{\text{solution}}} \cdot \left(\frac{\text{mL}_{\text{solution}}}{0.915 \text{g}_{\text{solution}}}\right) = 4.92\% \text{ m/m}$ Watch the units! Keep them straight or you'll convert upside down!

Now we are at a GOLDEN point!!! When we have m/m, we can separate solute from solution to get solvent! This is needed for molality and mole fraction. To wit....

There are 100 grams of solution and 4.92 grams of it are solute. Therefore, the grams of solvent (water in this case) is...

 $g_water = 100 \cdot g_solution - 4.92 \cdot g \cdot glucose = 95.08 \cdot g \cdot glucose$

Now we have grams of solute and solvent and we can move to the remaining items...

There are.. $\frac{4.92 \cdot g_glucose}{95.08 \cdot g \cdot solvent}$ Thus, adjusting the units for molality, we have...

 $\frac{4.92 \cdot \text{g}_{glucose}}{95.08 \cdot \text{g} \cdot \text{solvent}} \cdot \left(\frac{1000 \cdot \text{g}_{solvent}}{\text{kg}_{solvent}}\right) \cdot \left(\frac{1 \cdot \text{mole}_{glucose}}{180 \cdot \text{g}_{glucose}}\right) = \frac{0.287 \cdot \text{moles}_{glucose}}{\text{kg}_{solvent}} = 0.287 \cdot \text{molal}_{glucose}$

We can now use the known grams of solute and solvent for mole fraction. We know that there are...

 $\frac{4.92 \cdot g_glucose}{95.08 \cdot g \cdot water + 4.92 \cdot g_glucose}$

All that is needed is to convert the grams to moles...

$$4.92 \cdot g_glucose \cdot \left(\frac{1 \cdot mole_glucose}{180 \cdot g_glucose}\right) = 0.0273 \cdot moles_glucose$$

95.08 \cdot g_water $\cdot \left(\frac{1 \cdot \text{mole}_water}{18.0 \cdot \text{g}_water}\right) = 5.28 \cdot \text{mole}_water$

All we need to do is to replace the grams by the respective moles!

$$X_{glucose} = \frac{0.0273 \cdot moles_glucose}{5.28 \cdot mole_water + 0.0273 \cdot moles_glucose} = 0.00514$$

Finally, the ppt and ppm are simple. Just take the respective values (m/m or m/v) and multiply as needed..

ppt (m/m)	A thousand is 10 times 100. So ppt m/m is 10 times % m/m!
	ppt = $10 \cdot (4.92 \cdot \%) = 49.2$ Simple!!!
ppm (m/v)	A million is 10,000 times 100, so ppm m/v is 10,000 times % m/v $$
	$ppb = 10,000 \cdot 4.50 \cdot \% = 45000$ Tada!!

Example 2: Here, I'll start with a less conventional unit and work backwards.

Consider a $X_{KF} = 0.125$ solution of KF (MW=58.1). If it has a density of 1.00 g/ml, calculate Molarity, molality, %m/v and %m/m.

This one is tricky to get started. The key is to understand that <u>a solution is a relative ratio of</u> <u>solute to solution or solvent, thus the concentration is independent of the amount of</u> <u>solution that one has!</u> This means that if I have a mL, a gallon, or a tanker full..the concentrations do not change!

Why do I mention this?? Because I'm going to take advantage of this by defining an amount of solution that is convenient for me. (It's is all about me, of course.)

To start, I'll select 1 mole of total solution. Thus by definition of mole fraction, I can calculate the moles of water.

 $1 \cdot \text{mole}_\text{solution} = \text{moles}_\text{KF} + \text{moles}_\text{water} = 0.125 \cdot \text{moles}_\text{KF} + \text{moles}_\text{water}$

Thus...

moles_water = 1.00·moles_total - 0.125·moles_KF = 0.875·moles_water

Now, simply work backwards from Example 1...Since $X_{HF} = 1$, we write that there are

 $\frac{0.125 \cdot \text{moles} \cdot \text{KF}}{0.125 \cdot \text{moles} \cdot \text{KF} + 0.875 \cdot \text{moles} _ \text{water}}$

Convert to grams now. (Note that this is the reverse of the last example)

$$0.125 \cdot \text{moles}_{KF} \left(\frac{58.1 \cdot \text{g}_{Kf}}{\text{mol}_{KF}} \right) = 7.26 \cdot \text{g}_{KF}$$

$$0.875 \cdot \text{moles_water} \cdot \left(\frac{18.0 \cdot \text{g_water}}{\text{mol_water}}\right) = 15.75 \cdot \text{g_water}$$

That being done, let's calculate % m/m and then molality..

%m/m $\frac{7.26 \cdot g_KF}{7.26 \cdot g_KF + 15.75 \cdot g_water} = \frac{0.316g_KF}{g_solution} = \frac{31.6 \cdot g_KF}{100 \cdot g_solution} = 31.6\%$ %m/m

and molality..while we're here.. $\frac{0.125 \cdot \text{moles}_\text{KF}}{15.75 \cdot \text{g}_\text{water}} \cdot \left(\frac{1000 \cdot \text{g}_\text{water}}{\text{kg}_\text{water}}\right) = 7.94 \cdot \text{molal}$

Now, remember the golden hint above??? Use it in reverse now!!

$$\frac{31.6 \cdot g_KF}{100 \cdot g_solution} \cdot \left(\frac{1.00 \cdot g_solution}{mL_solution}\right) = \frac{31.6 \cdot g_KF}{100 \cdot mL_solution} = 31.6 \cdot \% \qquad \% m/v$$

WOW!! Note how, since the density is 1.00 g/ml, the % m/m and % m/v are the same! This is true always. It's also good to remember that if the density is close to 1.00, say 1.06 g/ml, then the % m/v and % m/m will be very close to each other.

Now, let's do the reverse of what we did in the first Example where we converted from Molarity to % m/v.

$$\frac{31.6 \cdot \text{g}_{KF}}{100 \cdot \text{mL}_{\text{solution}}} \cdot 10 = \frac{316 \cdot \text{g}_{KF}}{1000 \cdot \text{mL}_{\text{solution}}} \cdot \left(\frac{1 \cdot \text{mol}_{KF}}{58.1 \cdot \text{g}_{KF}}\right) = \frac{5.44 \cdot \text{mol}_{KF}}{\text{L}_{\text{solution}}} = 5.44 \cdot \text{M}$$

Hopefully, with practice, you will see that there is a pattern to all of this. Once you become familiar with the pattern (like knowing the pattern of roads in your neighborhood), you'll perform the steps easily.