

Quantitative Methods in Chemistry
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Lecture-04
Relationship Between Various Concentration Parameters

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Parameter	Units	Temp./Density	Mol. wt(?)	Interconversion
Molarity	M (mol L ⁻¹)	Temp. depen	✓	$M = \frac{n}{V(L)}$
Molality	m	Temp. Indepen	✓	$m = \frac{n}{w(kg)} = \frac{n}{V \times \rho} = \frac{M}{\rho}$
Normality	N	Temp. depen	✓, neg.	$N = M \times n\text{-eq.}$
% mass/vol	% w/v	Temp. Indepen	✓	$= \frac{w \text{ (mg)}}{V \text{ (mL)}} \times 100$
% vol/vol	% v/v	Temp. depen	X	
parts per million	ppm mg/L		X	w/w v/v
parts per billion	ppb µg/L		X	
p-value	unitless	Temp. depen	✓	$pX = -\log [X] \rightarrow \text{Molarity}$
mole fraction	unitless	Temp. Indepen	✓	$X_i = \frac{n_i}{\sum n_i}$

Welcome to the 4th lecture in the first week of quantitative methods in chemistry. Let us start by summarizing or rather comparing the different units of concentration that we have discussed in class so far. So I am going to make a large table. Hopefully that is going to help us understand what is how things go. So first one is the parameter. Next one, let us call it units. Followed by temperature, then see to understand whether it require is it independent of measurement of temperature.

Then we can try to understand how this can be interconvert it, does it require molecular weight interconversion okay. So, let us keep the basis of everything as molarity that will help us related across different units. So the units of molarities capital M molar and is the temperature independent then dependent largely because you have volume in the denominator, which will change as a function of temperature or other which could changes function of temperature.

Yes, it requires the molecular weight to be known to be defined. So, basically molarity is defined as number of moles divided by volume of solution in liters. And this is also given as moles per liter. So, keeping this as the reference standard, let us go on to understand what is molality. This goes with the unit small m molal is a temperature dependent, then independent. Does it require a knowledge of molecular weight yes.

And m is defined as n divided by weight in kgs and how would you convert weight is that you are going to go number of moles divided by volume times density of solution. So, basically this is nothing but molarity divided by the density of solution, the next unit is normality. Normality is given capital N and this is temperature dependent. Yes, it does require the knowledge of molecular weight and the concept of equivalence.

And how does this go. Normality as we have seen before, is the product of molarity does a number of equals. Remember to define normality you have to define what reaction you are going to be using the chemical under. The next series of measurements the parameters are percentages. So, we have mass percent, which goes unit less basically you have percentage weight by weight is how it is defined.

You also have percentage volume by volume. Then you have percentage weight by volume. Mass volume only weight by weight is temperature independent. While these 2 are temperature dependent, none of this required the molecular weight to be known for the chemical that you are working with. Just for weight by weight, one is able to understand so let us go weight by weight it is going to be given by weight of solute in grams divided by weight of solution in grams times 100.

I am not going to end up converting this but we are able to realize that at the denominator, you have something similar to morality, I am pretty sure you will be able to sit down and finish how to convert this to the other, it is going to involve densities that go with it. And also conversion entity that comes from grams to kilograms and to liters. Similar would be the others as well. So the other entity that we saw here was parts per x. So this could be parts per million or billion.

So this also goes as ppm and ppb and ppm roughly translates into 1 milligram per 1 liter. On the other hand, ppb goes as 1 microgram per liter. In this case, its temperature independent to start with, because you have the denominator as the mass of the solution. But however, that does get changed into the volume of solution. So, the temperature dependence here depends upon the denominator that you go if it is volume, it is going to be independent, you do not need the knowledge of what is the molecular weight.

And of course, this once again goes very close to weight by weight type of a definition, or even made by volume. So the conversion go in such a fashion. There is also the parameter the parameter p value or the p function, which is unit less. This is nothing but negative logarithm of concentration of x in molarity. So, there you go is the direct interconnection from molarity to p x is this temperature dependence. Since molarity is temperature dependent, yes this is temperature dependent.

And also it requires the knowledge of molecular weight, to finish with we have mole fraction, mole fraction is also unit less it is temperature independent, it does require the knowledge of what is the molecular weight of the concerned chemicals and the interconversion molarities not that straightforward but basically what we are able to understand the mole fraction of any constituent i is going to be going by the number of moles n_i divided by some of the number of moles of all the entities that are present within the solution.

Now that we have seen all the definitions for these different parameters to determine concentration. Why do not we go ahead and take up an example in this case.

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30% w/v of methanol in water @ 20°C

$\rho_{\text{soln}} = 0.952 \text{ g/cm}^3$
 $\rho_{\text{MeOH}} = 0.792 \text{ g/cm}^3$
 $\rho_{\text{H}_2\text{O}} = 0.998 \text{ g/cm}^3$

30g of MeOH in 100ml soln.

$M_{\text{soln}} = \rho_{\text{soln}} \times V_{\text{soln}} = 0.952 \times 100 = 95.2 \text{ g}$
 $\Rightarrow (95.2 - 30) \text{ g} = 65.2 \text{ g of water}$

$\text{w/w} = \frac{30 \text{ g}}{95.2 \text{ g}} \times 100 \% = 31.5 \% \text{ w/w}$

v/v 30g of MeOH $V_{\text{MeOH}} = \frac{M_{\text{MeOH}}}{\rho_{\text{MeOH}}} = \frac{30 \text{ g}}{0.792 \text{ g/cm}^3}$
 $= \frac{37.9 \text{ mL} \times 100\%}{100 \text{ mL}} = 37.9 \text{ mL}$
 $= 37.9 \% \text{ v/v}$

$30\% \text{ w/v} = 31.5\% \text{ w/w} = 37.9\% \text{ v/v}$

So let us take an example of 30% weight by volume of methanol in water, and determine what is its molarity, molality and normality 8% percent definition of weight by weight volume by volume or weight by volume, the few parameters that would be required in this case are density of solution is point 952 grams per cc density of methanol is 0.792 grams per cc and density of water is 0.998 grams per centimeter cube.

All these values are at 20 degrees Celsius. So now to start with let us convert weight by volume to weight by weight and how does this go. So, this first implies you have 30 grams of methanol in 100 ml of solution, 100 ml of solution would indicate that what is a mass of solution this will be equal to density of solution time volume of solution, density of solution is point 952 grams per cc times 100 ml. So that is going to make it 95.2 grams.

So, this indicates if 30 grams is methanol, how much of water is present. This is going to be 95.2 - 30 grams = 65.2 grams of water right. So now what ends up happening for underdetermined what is weight by weight, what is the total is 30 grams divided by 95.2 grams times 100% = 31.5% weight by weight. So now comes to the next conversion. Let us look at volume by volume. In this case you are trying to say you have 30 grams of methanol.

And in order to understand what is the volume of methanol, you have to take the mass of methanol and divide it by density of methanol. So, this will end up to be 30 grams divided by

density of methanol is 0.792 grams per centimeter cube. So, this will be equal to 37.9 ml. So, therefore, the volume by volume is going to be equal to 37.9 in 100 ml. This will be equal to 37.9% volume by volume.

So we are able to understand 30% weight by volume = 31.5% weight by weight = 37.9% volume by volume. So be very careful when you are expressing your concentration units in percentage without the units it does not make sense.

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The slide contains handwritten calculations for the concentration of a 30g methanol solution in 100ml of water. It includes the following steps:

- Moles:** $n = \frac{30g}{32g/mol} = 0.9375 \text{ moles}$
- Molarity (M):** $M = \frac{0.9375}{0.1L} = 9.375 \text{ M}$
- Volume (V):** $V = 100 \text{ mL}$
- Mass (M):** $M = V \times \rho = 100 \times 0.952 = 95.2 \text{ g}$
- Normality (N) for complete reaction:** $N = M \times 3 = 28.125 \text{ N}$
- Normality (N) for incomplete reaction:** $N = 9.375 \text{ N}$
- Mass of water:** $95.2 \text{ g of water} \times \frac{18}{18} = 95.2 \text{ g}$
- Molarity of water:** $\frac{95.2}{18} = 5.29 \text{ moles}$
- Molar Fraction of Methanol:** $X_{\text{MeOH}} = \frac{0.9375}{0.9375 + 5.29} = 0.151$
- Molar Fraction of Water:** $X_{\text{H}_2\text{O}} \approx 0.849$

Chemical reactions shown for normality determination:

- Complete reaction: $\text{CH}_3\text{OH} + \frac{3}{2}\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O}$ (oxidation state change from +1 to +4)
- Incomplete reaction: $\text{CH}_3\text{OH} + \text{O}_2 \rightarrow \text{CO} + 2\text{H}_2\text{O}$ (oxidation state change from +1 to +2)

Now let us move ahead to determine what is the molarity. So what did we say 30 grams of NaOH, so how many moles is this number of moles is given by a CH₃OH that will be 12 + 4 + 16 32 grams per mole. So when you have 30 grams divided by 32 grams per mole, this is going to be equal to 0.9375 moles. So, therefore the molarity will be equal 0.9375 divided by 0.1 liters, which is going to be 9.375 molar.

Moving on what is the molarity, molarity is going to be given by 0.9375 as we know volume is 100 ml and you need to convert it to mass, the mass is going to be given by volume times density, 100 times density was 0.952. That makes it 0.0952 is going to be equal to 9.847 molar. Now to understand which reaction we are going to determine normality for. Let us take for an example, we are doing combustion of methanol.

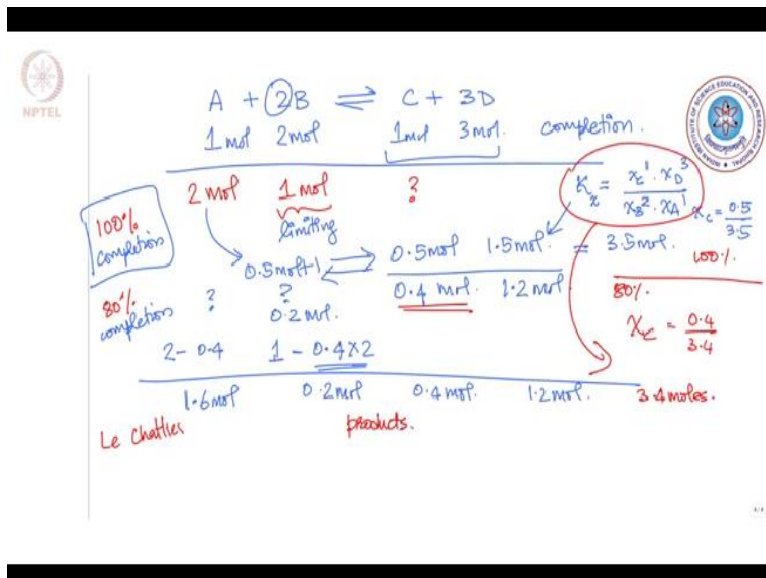
In combustion of methanol, methanol reacts with oxygen. Let us assume complete combustion, we can also do the normality for incomplete combustion a moment later, complete combustion will give you carbon dioxide. So this has to be equal to 3. So let us make it 3 by 2. So, once you have something like this, the important thing to understand here is that the oxidation number of carbon in this case is 1.

On the other hand, it goes to + 4, therefore, 3 electrons are involved. For complete combustion, 3 electrons are involved. So therefore the normality is going to be given by molarity times 3 28.125 normal. On the other hand, if you are doing an incomplete combustion which is $\text{CH}_3\text{OH} + \text{O}_2$ giving carbon monoxide + H_2O . This is already balanced and here what ends up happening is that oxygen goes to something like a + 2 oxidation state from + 1 here normality will be equal to molarity.

What one is able to understand here the normality determination request and knowledge of what kind of reaction has undergone by methanol to define what is the normality okay, so now we could always define what is the p in methanol but since the concentration is so high, generally p is determined. Generally p value is always associated with lower concentrations of solute. Let us say determine what is the mole fraction we just determined the number of moles of methanol is 0.9375.

In this you also have 95.2 grams of water 95.2 divided by 18 will be number of moles of water that is going to be equal to 5.29 moles. So, the mole fraction of methanol is going to be equal to 0.9375 divided by $0.9375 + 5.288$, this will be equal 0.151 and therefore, H_2O will be approximately 0.849. So, what we have seen here is that the mole fraction although you have significant amount of methanol is actually lower because you are dividing it by the molecular rate. And the remaining is being water, you have significant amount of water that is present.

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Let us switch a few beers. And let us try to understand this documentary a little bit more. Now that we have defined all the different concentration units. Let us take a simple reaction of $A + 2B$ that results in an equilibrium of $C + 3D$, that the numbers in front indicate their stoichiometric equals okay. Now that you have something like this, so what we are able to understand here if you have one mole of A that requires 2 moles of B to be 1 mole of C, and 3 moles of D.

Now the question is this is under the assumption that the reaction goes to completion. So for this reaction that has been given here, let us take an example where instead of giving the stoichiometric proportions, you give non stoichiometric proportions. This many times happens when you are starting out to the reaction being unsure of water, it is stoichiometric equivalents. So for instance let us say you provide a 2 moles of A and 1 mole of B.

And then you are trying to ask how much of C is going to be made. Once again, let us assume 100% completion. So what is going to end up happening here, in this case, the B is going to be the limiting reagent and you realize for 2 moles of B, 1 mole of A is going to be required. So out of this 2 mole, you are only going to end up using 0.5 moles. And since both these 2 moles are going to be used, you are going to make 0.5 moles of C and 1.5 moles of D.

This is once again assuming 100% conversion. What could end up happening here is that it does not have to end up in a complete conversion to C and D, it could be in an equilibrium where you

form less of C and D. For instance, let us assume 80% conversion happened and you have 0.5 mole of C, then can we ask a question how much of A or B are remaining under such a case.

So, as I just mentioned, you started with 2 mole of A and 1 mole of B to get 0.4 mole of C. So in this case, we are talking about 80% completion. So in that case what ends up happening, you are able to realize 3 equivalents of D is going to be coming up, so this is going to be 1.2 moles. And on the other hand, if only 0.4 got used up, you are going to have 0.2 moles of B remaining. How did I calculate this.

I calculated this as $1 - 0.4 \times 2$, 2 comes from the fact that you have 2 equivalents of B that is required, and 1 is the initial concentration of B that was provided. And out of the 2 moles that you started with, you are going to end up with $2 - 0.4$. So you are going to have 1.6 moles of A 0.2 moles of B remaining with 0.4 moles of C and 1.2 moles of D being prepared. So what we have seen here is that how does the equilibrium constant change.

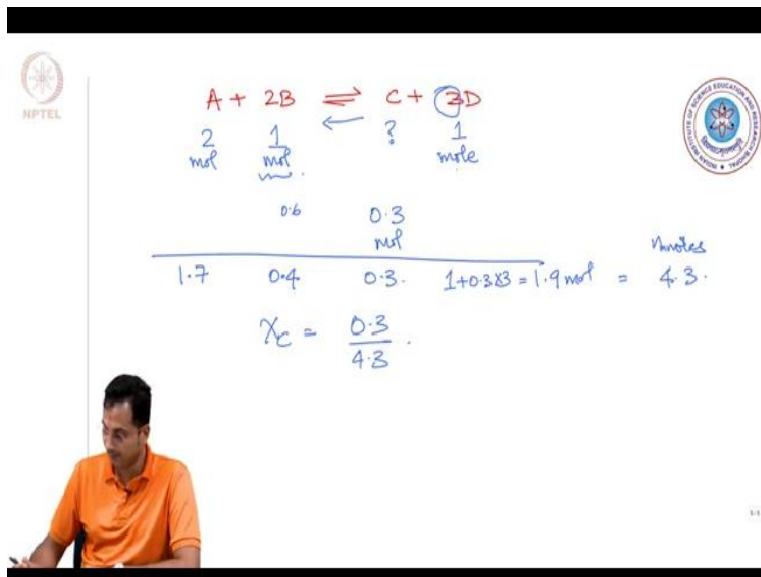
In this case, of course, you assume complete completion of reaction where the equilibrium constant would have been given by in this case, it would have been given by let us say we are going with the mole fraction. The mole fraction indicates a K_{chi} that we are trying to calculate And then the number of moles as a sum, you are going to get something to the order of $1.5 + 1 + 2$, that is going to be 3.5 moles being the total.

And then your K_{chi} is going to be given by chi_c to the power 1 chi_D to the power 3 divided by chi_B to the power 2, and chi_A to the power 1 right. So now this has happened, what is chi_C , in this case, chi_C is going to be given by 0.5 divided by 3.5. Once again, what I am assuming here, this is the equilibrium constant for the 100% completion, what you are able to realize, on the other hand, if you have an 80% completion, the total number of moles is going to be the sum of $1.6 + 0.2$ which is $1.8 + 0.4 + 1.2$.

That is going to be 3.4 moles. In this case, your chi_C is going to be 0.4 or 3.4. But the value of chi_C chi_D chi_A and chi_B are going to change with results in a different equilibrium constant. So basically one has to be a little careful calculating equilibrium constants. Let us try to push this

a little bit by using the Le Chatelier principles. So in this principle, you know for a fact that if you are adding some of the products, the equilibrium constant is going to be pushed towards the reactants.

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So let us write the reaction again. 1 A + 2 B gives C + 3 D. And we took the example of having 2 moles here, 1 mole here. Nothing of C, now let us take for an example, you already had 1 mole of C, sorry, let us assume that you had 1 mole of D that you have already provided. So what this will end up doing is it is going to push the reaction towards more towards the reactants. Let us assume that in this case, what you have been able to determine that C is present in 0.3 moles after the reaction gets over.

And what you are able to understand here is that this immediately implies you use the 0.6 here, so you are going to have 0.4 remaining, and 1.7 of A remaining and B is going to be 1 + 0.3 times 3 because you have 3 equivalents of it, that will be 1.9 moles. Once again, going back you have a total number of moles, which is going to be equal to 1.7 + 0.4 + 2.1 + 1.9 is 4.3 moles.

Now chi C is 0.3 by 4.3. What you are able to realize once again in these examples is that the equilibrium constant helps you understand how much of the reaction was forward and in these 3 different conditions, but in condition one you assumed 100% completion with non stoichiometric amounts of reactance. And with 80% completion, once again, the similar non stoichiometric

amounts, you are able to realize the equilibrium constant defined by K_c is different from one another.

Similar is an example where if you also provide a little bit of the product being present, that is the difference that comes in the equilibrium constraint that is determined. So one is able to understand providing an idea of how much reactants and products you have and the equilibrium constant helps you judge how much forward has the reaction gone. These examples help you understand how stoichiometry works in different chemical reactions under different conditions that have been set up by the researcher.

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The whiteboard contains the following handwritten notes:

$pX = 13.5$ units. Molarity = ?
 $pX = -\log [X] \rightarrow$ molarity
 $-13.5 = +\log [X] \quad [X] = 10^{-13.5}$
 $[X] = 3.16 \times 10^{-14} \text{ M} = \underline{\underline{31.6 \text{ fM}}}$

The table of metric prefixes is as follows:

10^{12} - Tera T	10^9 - Giga G	10^{-6} - micro μ
10^6 - Mega M	10^3 - kilo k	10^{-9} - nano n
10^0 - 1	10^{-1} - deci d	10^{-12} - pico p
10^{-1} - deci d	10^{-2} - centi c	10^{-15} - femto f
10^{-2} - centi c	10^{-3} - mill m	10^{-18} - atto a

Let us take another example right now where if the pX for a given solute 13.5 units what is the concentration in molarity. So, pX is defined as $-\log$ of concentration of X in molarity. So, therefore, what is going to end up happening 13.5 is equal to $-\log$ of concentration of X . So, this transfers into -13.5 is equal to \log of X and therefore, X is going to be given by 10 power of -13.5 . So, the concentration of X is going to be given by 3.16 into 10 to the power of -14 molar.

Generally these kind of numbers which are coming as the 10 powers to certain numbers will be defined in different ways. For instance, 10 power -14 can be written as 10 times 10 power -15 . So, this will translate to something like 31.6 femtomolar. So let us take a quick look at these kind of numbers which might end up being extremely helpful for us. So let us start from larger

numbers, which we are more comfortable with, so why do not we put 10 power 0 as the reference that we are starting with.

So this is going to be 1. So something like 10 power 3 is given the unit kilo so that generally that is the one that comes with a small k 10 power 6 comes us as mega that is capital M 10 power 9 comes as giga which is capital G, 10 power 12 is tera with a capital T and so on and so forth. Let us go looking at smaller numbers 10 power - 1 is given as deci 10 power -2 is given a centi. We are very familiar with decimeter and centimeter 10 power - 3 is milli as a millimeters.

10 power - 6 then is micro, given the symbol mu 10 power - 9 gets the name nano, which goes to the small n, 10 per - 12 goes with pico with the small p, 10 power - 15 goes with femto, that is f that is what we ended up getting the current example and 10 power - 18 is atto which was a small a, there are many other units that could end up coming but these are the units that we might end up using most commonly and therefore has been introduced in this given example.