Quantitative Methods in Chemistry

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Lecture - 8
Error Propagation and its Application to a Few Examples, Significant Figures

Welcome to the next lecture in Quantitative Methods in Chemistry. In the last class, we tried to put some emphasis on understanding, how errors propagate, when you have multiple measurements that finally gives you one measurable. We tried to estimate how much error goes.

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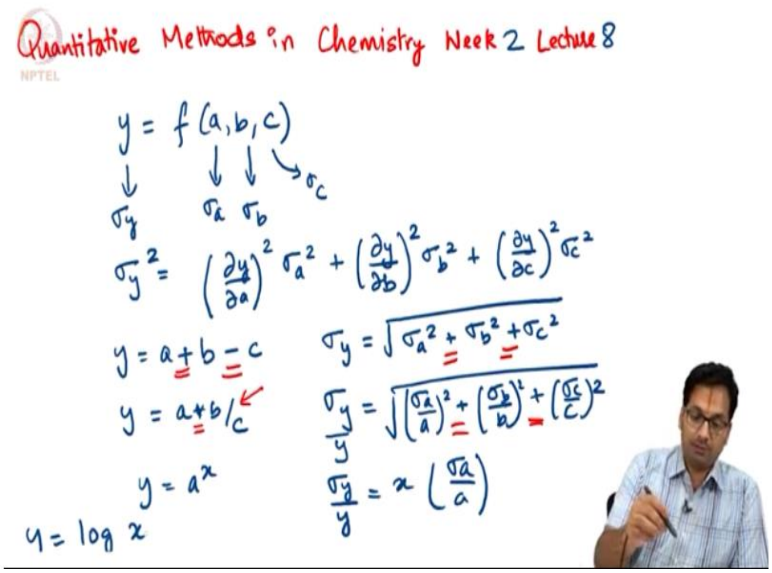

And this was done by using an equation, for instance you are trying to measure something like y that is a function of a, b and c. We derived the equation and let us say each one of this is associated with an uncertainty, then the overall uncertainty in sigma y is given as a square of sigma y square with the differential of each one of the variables, as shown here and after having done this, we applied it to a few simple examples.

Meaning that, when you have a sum and difference, how do the formulae differ? For instance, when you have y as a plus b plus, a plus b minus c, then what is the sigma y involved? That was given by sum of the square root. The uncertainty associated y in this case would be given as the square root of the sums of the squares of the individual uncertainties that is square root of sigma a square plus sigma b square plus sigma c square.

One has to remember that although this is a plus b minus c, all the errors accumulate with one another and other examples that we saw were something like a times b divided by c. In this case, sigma y is given as the sum of square root of, of course, sigma y by y, is given by sigma a by a the whole square plus sigma b by b the whole square plus sigma c by c the whole square. Once again, let me emphasize that irrespective as if there is a multiplication or a division there is a plus sign that goes here.

So now that we saw these two, I think we saw one more example which is y equal to a power x, in which case sigma y by y was given by x times sigma a divided by a. So these were the examples that we saw and the other example that were given to you as a problem was, what if you have y of log x. So we will see that in a moment.

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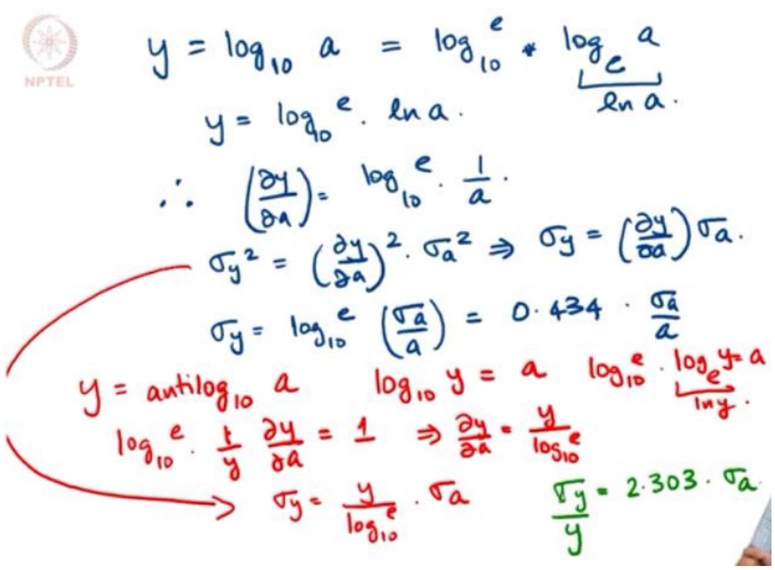

So in this example, we will be trying to see what is y equal to log of x. By default, when you say log, we mean log to the base 10. So in this case, let us make sure that we keep the notation constant. Let us say y equal to log 10 of a, then this can be rewritten as log e to the base 10, which will a constant times log a to the base e, which is nothing but ln a. Therefore, y is equal to log e to the base 10 to ln of a.

Therefore, dou y by dou a is going to be given by this constant log e to the base 10 times 1 over a alright. So now therefore, sigma y square is dou y by dou a the whole square times sigma a square. Since there is only one, so you can rewrite it as sigma y is equal to dou y by dou a times sigma a. Therefore, sigma y is going to be given by log of e to the base 10 sigma a by a. Log e to the base 10 incidentally happens to be 0.434 times sigma a by a.

Similar was the exercise that was given to you, which is y equal to antilog to the base 10 of a. In this problem, one can imagine, let us say we take a logarithm on both sides, log y to the base 10 will be equal to a and this also implies log e to the base 10 times log y to the base e is equal to a. This is nothing but ln of y. So that makes it easier for us to calculate. So log e to the base 10 times 1 over y dou y by dou a is equal to 1.

So this implies dou y by dou a is equal to y divided by log e to the base 10. So this once again, applying this formula here, what will end up happening sigma y will therefore be equal to y divided by log of e to the base 10, 10 sigma a. So therefore this becomes sigma y is equal to, sigma y by y is equal to 2.303 times sigma a. Now that we have seen these examples, let us try to solve some problems associated with it.

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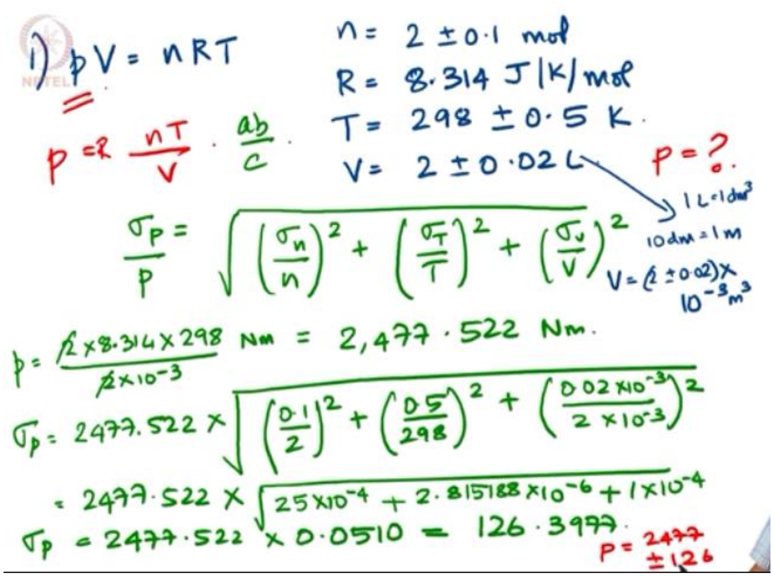

Let us take the first problem, which we can imagine as the ideal gas equation pV is equal to nRT. Let us say, that you want to determine what is the pressure in this case, provided the other constants are available with you. Let us say the number of moles is 2 plus minus 0.1 moles. One can ask where does the error for the number of moles come in, maybe it could be coming from the measurement. Let us say you are trying to take the weight of a gas.

So probably you have some error in its measurement of its weight or even the partial pressure that it might be exerting. So therefore errors do come across different variables that we end up using. Let us assume for now just for the sake of understanding that the universal gas constant is fairly accurate rather entirely accurate. Then, let us say the temperature is at 298 Kelvin, of course there is an error that is also associated with it.

Now let us say for a volume of 2 plus minus 0.02 liters, what is the pressure? You are able to realize for each one of these variable V is associated with a certain error. The number of moles is associated with a certain error, so is the temperature associated with a certain amount of error. So what would be the error associated with p is the question in this case. So let us try to solve this problem. So this can be quickly rearranged as p is equal to nRT by V and we realize that R is a constant.

So, one can always switch the constant out. So you can say R times n times T divided by V is what is the pressure and you realize this is of the example, where this is ab divided by c, alright. So let us determine what is the pressure the error that will be associated with the pressure. So this will end up as sigma p will be given by, of course sigma p by p will be given by square root of sigma n by n the whole square plus sigma T by T the whole square plus sigma V by V the whole square.

One thing I would like to convert is to convert the liters to an SI unit. So therefore one liter is 1 decimeter cube and 10 decimeters make a meter. So therefore, volume is nothing but 2 plus minus 0.02 into 10 to the power of minus 3 meter cube. This will help us get the pressure in SI units of Newton meter okay. So now that we have done this, let us calculate it really quickly. So p is going to be given. First let us actually determine, what is p by itself.

P is going to be given by 2 into 8.314 times 298 divided by 2 into 10 to the power of minus 3. So this will be in Newton meter, which is the SI unit of pressure. So that is going to end up as 2477.522 Newton meter. So now let us calculate what is sigma p. Sigma p now is going to be given by 2477.522 times 0.1 by 2 the whole square plus 0.5 by 298 the whole square plus 0.02 10 power minus 3 divided by 2 into 10 to the power of minus 3 the whole square.

So this finally reduces itself. Once we are able to do the arithmetic, you see the sigma p associated is about 126.4 units and then the final way of reporting this value would be the pressure is nothing but, in this case, 2477 plus minus 126 would be the way a person would be providing the value. So basically the answers uncertainty associated is in the last 3 digits and we are able to see the same thing, meaning that these three digits are uncertain.

And we understood what kind of uncertainty has come up when you have a distribution of values and this kind of helps you understand the distribution that is associated with sigma p in this given case. Let us take another example to understand and exemplify the same case further with a simple arithmetic.

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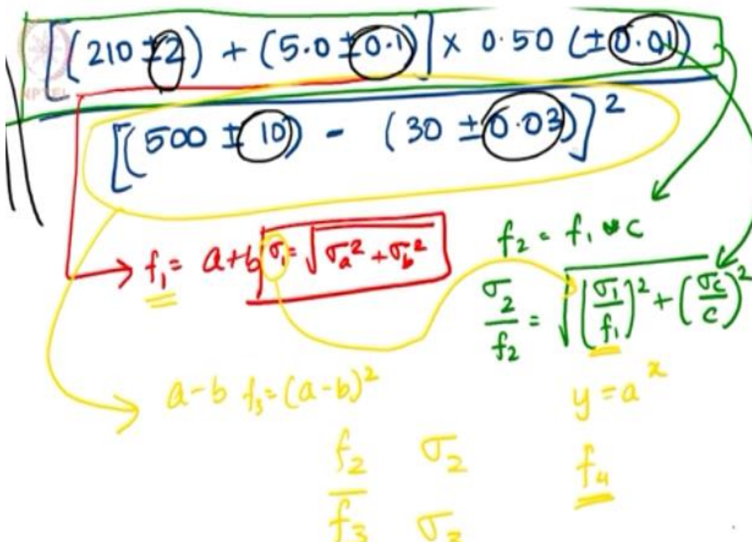

Let us try to calculate what is 210 plus minus 2 plus 5.0 plus minus 0.1 the whole multiplied by 0.50 plus minus 0.01 divided by, so this seems a little involved, but let us just break it into multiple pieces. This is one piece, this is the other piece, this is the third piece and all these pieces put together will be the entire fourth piece that will help you understand what is the deviation that comes in.

So I am going to leave it to you as an exercise, but what I would like to do is to break it down to pieces, so that we understand. The first piece one is able to immediately understand is nothing but a plus b and here we know for a fact that the error goes the sum of squares of the deviations for each of the measurement. So let us, say I am going to call it f1 just for the sake of simplicity. We see that the next calculation f2 is f1 times c.

That is what we are seeing here, in which case sigma 1 is going to be given by this and sigma 2 by f2 is going to be given by square root of sigma 1 by f1 the whole square plus sigma c by c the whole square and you have sigma c from here and the sigma 1 will arise sigma 1 will be fed from this case and of course f1 is determined in this case already by the sum of 210 + 5 and on the other hand, what you are able to see at the denominator?

Denominator has two different functions that are going with it. The denominator has something like a minus b and on top of it, you also have a a minus b the whole square. So you are going to be exploiting the formula, such as y equal to a power x and then finally once, let us say this is f3 once you have gotten f2 and f3 you are having something like f2 divided by f3 and each of this is associated with a certain error. So finally, you will be able to get what is f4.

Let us say, that is where we started with. So f4 will be given by the sum of all of these different errors. Sum in the sense like, the way you determine each one of this sigma, final Sigma that is associated with f4 will be the overall measurement. So this is a problem, that is given to you, which we will see the answer for in the next class. So one is able to understand if there are small errors associated each of the measurement, what is the overall error that comes up?

It is not based on what is the large number, what are the number of decimals that one sees, but by properly doing error propagation. So this takes us to the concept of significant figures. So let us quickly look at what significant figures are?

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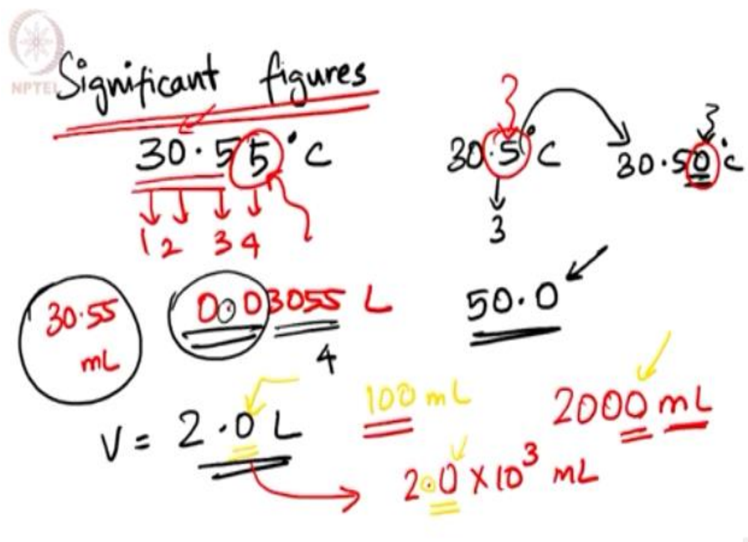

So significant figures, for instance, let us say you are providing something like 30.55 degree celsius. So how many significant figures are here? One would say that there are four significant figures. On the other hand, one has to be careful about how zero comes into play, if I had given the same thing as 30.5 degree celsius, we would only say there are three figures. However, you can always add a zero here and say 30.50 degree celsius.

But if the zero is indicated, it could imply something in the sense that that is lack of precision only in this digit. On the other hand, in the case of 30.5, we say the lack of precision is in this digit and in this case we are saying the lack of precision is in this digit. So basically significant figures are numbers that are expressed in terms of whatever is certain and with the last digit that is uncertain. One has to be very careful on using zero.

So instead of using 30.55 degrees celsius, let us say you have 30.55 ml, one can always express 30.55 ml as 0.03055 liters. So in this case, you are having leading zeros that come up. One could always argue saying that do these form a part of significant figures, the answer is no. It is just used to establish where the decimal point is. So therefore it still remains as four as the number of significant figures. On the other hand, let us say somebody is clearly trying to say 50.0.

This indicates that the uncertain digit is in the last decimal as it is given here. So many times for something like in the case of volume, let us say somebody says you have a 2.0 liter in the volume. We just saw an example where pV equal to nRT was utilized to understand how to determine the uncertainty in pressure. In this case, let us say the volume is given as 2.0 liters. This clearly indicates the uncertainty is in the hundreds of milliliters.

So this matters a lot for one to understand, where the error comes in. Now on the other hand, if the same student ends up writing this as 2000 ml, this is in some ways misleading, because here you realize, you are talking about 100 ml error that comes in this decimal; however, in this case you are trying to say the same number that is rewritten as a 1 ml precision. So this is a problem. So what people end up generally writing is that they will write 2.0 times 10 to the power of 3 ml.

This is called scientific way of reporting in numbers, scientific format. So here, the point decimal helps you establish the error is here and not in this decimal. So significant figures are things that people end up using quite commonly to display their data.

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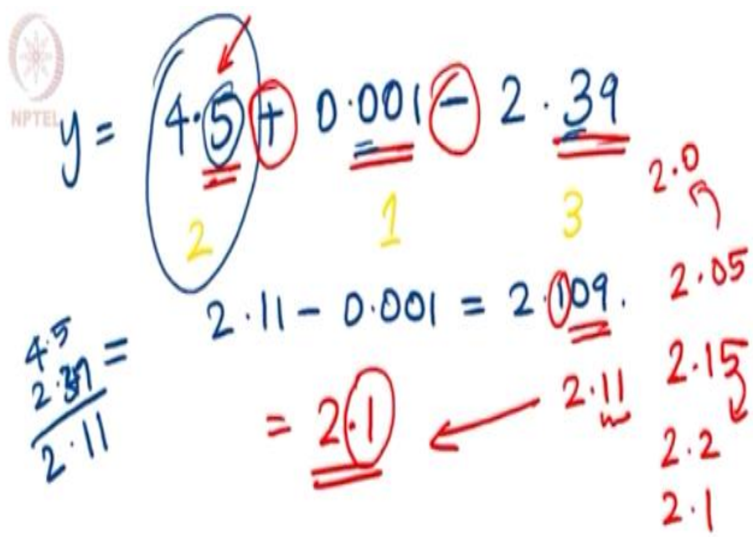

So let us take the example of where you are trying to calculate 4.5 + 0.001 – 2.3. One is able to appreciate the fact that this has a single decimal followed single digit after the decimal. This has three digits after the decimal and this let us say has two digits after the decimal. So significant figures for these are quite varying. So this is two significant figures, one significant figure and three significant figures.

So let us assume that these are all volumes that we are trying to measure and we are trying to take a sum or difference with respect to each one of them and we are able to realize that the maximum uncertainty is associated with this meaning that within the first decimal itself, the value changes. So now what is going to end up happening is that, 4.5 – 2.4 is 2.1, of course, we have to add one more to it, so it is going to be 2.11- 0.001, which is going to be 2.109.

So if you are able to realize, this is the answer that we get out of this arithmetic, but since the uncertainty is associated with a first digit, one has to express this value as 2.1. So we are able to understand that although different values come up, this is one way of scientific reporting that is given the term significant figures. So you are able to understand whichever has the least precision drives how many digits are expressed in the final value.

So generally numbers are rounded up. In this case, this would get rounded up to 2.11 and then what is going to end up happening is that this gets rounded up to 2.1. The controversy comes when you are having 2.15 and whether you should round it to 2.2 or 2.1. So generally it has done such that the next the even number is what is the round off done to, meaning that 2.15 will get rounded to 2.2, while 2.05 will get rounded off to 2.0.

So if this is done, the basic assumption here is that there are equally likely numbers that come close to the even and odd ones and therefore the average will properly be represented by the digits that are being measured in a given experiment.