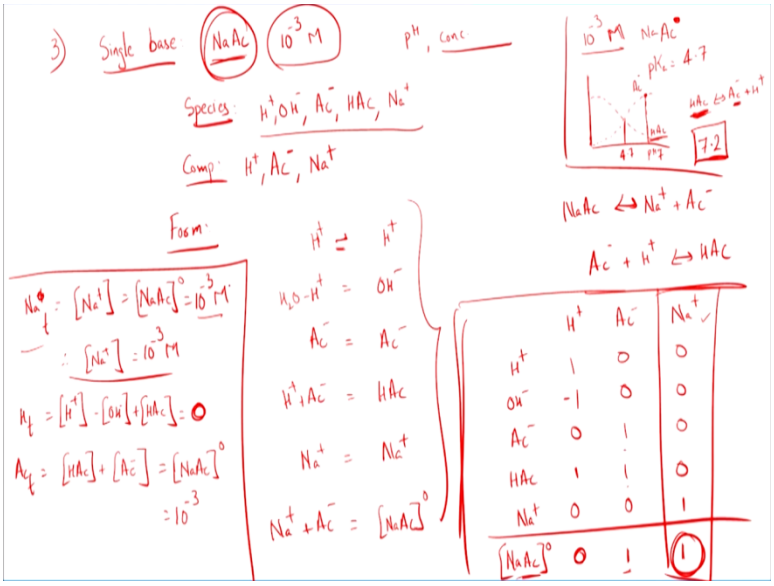
Environment Engineering: Chemical Processes
Prof.Dr. Bhanu Prakash Vellanki
Department of Civil Engineering
Indian Institute of Technology – Roorkee

Module No # 04
Lecture No # 18
Estimation of pH using VMINTEQ

Hello everyone back to our latest session i guess so we introduce ourselves to a new software visual MINTEQ and what is that give an idea about and how does that help us. It is going to help us in solving multiple equilibrium related scenario's right what are the concentration of your relevant compound at equilibrium let us say but for what do we able to develop. We need to be able to identify the components and also be able to give are specify what is the total component concentration going to be right?

So in that case in the previous lecture I believe we looked at case of adding a single acid to a bottle. So the next case we are going to look at again in a simple case I guess is going to be adding a single base to water right. So again the whole part of this class is not just to understand the system but also to be able to intuitively come up with the solution right so once we have relevant back ground we should be able to hopefully you know guess at the relevant answer. So that is something again we are going to try to in this particular class or session again right.

(Refer Slide Time: 01:34)



So let us see what we are here so the next example I guess we are going to have is that you know we are going to add a single base and what is that in this case earlier we looked at the single acid so we are going to use the conjugate or similar acid here and it is going to be NAAC or I guess sodium hastate and we are going to add it 10 power -3 molar and what to know the PH and the concentration of all and any other compounds that are going to be in solution right.

So earlier we had an acid and we looked at calculating the PH I think we are relatively decent job with respect to estimating the PH same here we try to let us try to estimate the PH of the solution now right. So the first is going to be a test for us I guess so let us to that here so we are adding 10 power -3 molar right not too strong or not too dilute either for the total is 10 power -3 molar and the not adding the acid here we are adding the base NAAC let us say.

So keep in mind now the PKL value is around 4.7 so let us look at the PH let us say right and we know that it is going to be something like this and if it is going to be something like this let us say and here I 4.7 so if you are adding base to water first the PH should increase it should hopefully be greater than 7 let us say right it is going to be greater than 7 what else can we look at let u say and that if it is 7 though or greater than 7 you see that most of it going to stay as AC – and little of it will probably be as HAC 4.7 and 6.7.

So very literal of it is going to be staying as HAC what is it mean so HAC and AC- and H+ right so when we are adding AC – to solution which is the case here very little of it going to be HAC as in very little H+ as going to be removed from your solution right so what is that mean the Phis going to slightly increase so let us say we are going to go with 7.2 maybe so this is my guess here.

Let us see or let us check later on I guess so let us come back to what we are here so first what is our approach here we always look are the species what is our approach here let us try to regurgitate you species we need to identify what are the compounds that are present at equilibrium in the solution and for this you obviously need some back ground and what is the background that we have some background with respect to acid and base chemistry right and we already discussed the relevant aspects so we do not need to go in that great detail.

So we identify the species that choose the component accordingly then write the formation equation pardon me and then come up with tableau and then the component balance equations and then we come up with equilibrium equation and then finally solve them. So obviously the V MINTEQ can Bi pass most of these but you at least be able to write the tableau or come up with the component balance equation right.

So let us see what we have here right so species now are going to be certainly H+ and OH – right so we are always going to have them water and whenever we have water these are aqueous solutions and then we have the deprotonated form AC- which is what we are adding and we are going to have protonated form HAC. So you are not sure that is why you are going to have HAC here I am not yet sure if we are going to have HAC or significant levels but we are going to go with having it.

And obviously because I am adding sodium I am also going to have NA + so what is the equation here I guess that we need to look at NAAC will dissociate into NA+ AC- NAC- + H+ which can go to H HAC that is what more or less looking at right so these are our species so what are out components similar to the last case we are going to choose how do we choose components always try to choose such that you know you are going to arrive the solution at earlier.

And in that case we say always choose H+ you can choose OH+ but you arrive at the solutions ahh later I guess actually working out by hand. And especially if you look a VMINTEQ I guess you would obviously try to choose H+ why I believe H+ is listed as one of your components right so again even if you are trying to work out by hand it is always better to choose those components that are given as preset components in your VMINTEQ so that is always a guaranteed way to arrive at your solutions fast.

So let us see here the components are going to be H+ and the thumb rule is most deprotonated form AC- and we are not done with that and still we need to form NA- we are going to go with and NA + and now the formation equations the formation equations what are they I guess I am going to list all my species here H+ OH- AC- HAC and NA+ and let met look at that how many

H+ need here 1H + to form = H+ H2O-H+ = OH- 1 AC - = form 1AC- and H+ +AC- will form HAC and 1NA+ will form my NA+.

Now I can come up with my tableau and what is my tableau here please and here I am going to have the components H+ AC- at NA+ and the relevant species here H+ OH- AC- HAC and NA+ and then here are species what did we add initially we have source compound for everything as NAAC and that is going to NAAC naught even for that I am going to write down NAAC naught how do I form that NAA+ + AC – NAAC naught.

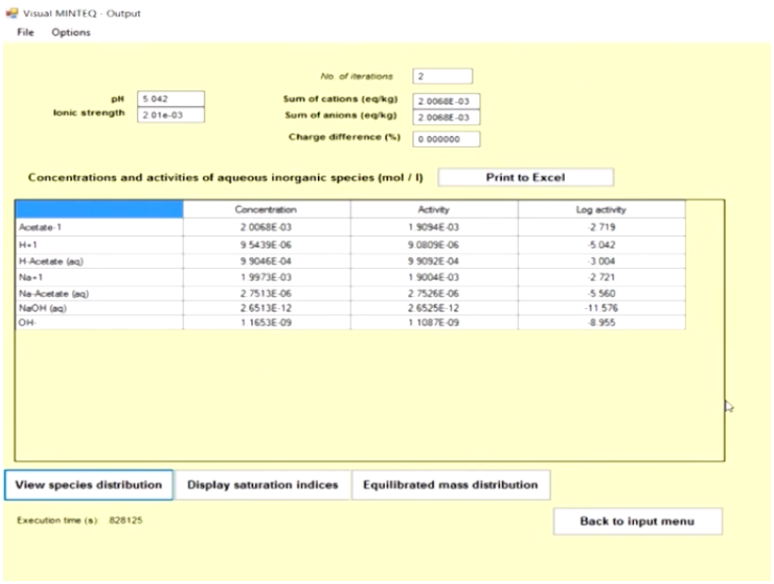
So anyway coming back here so first I am going to write the component to H+ in this formation equations right 1 H+ - 1010 and more critically 0 here right and AC- 00110 and again 1 here and here NA+ no for the role here at just a salt here so 1 and 1 right. So obviously you can straight away solve for concentration of NA + right if you apply.

So let us move on to this particular space here on left hand side and if I want to I can directly remove that particular variable from annual NA+ or NA total I am going to do the component balance here and here going to start with NA total = the concentration of NA+ at equilibrium and that as I see = 1 times NAC naught NNAC naught and that as an NO 10 power -3 molar. So concentration of NA+ should be equal to 10 power -3 molar.

So already done with that so I can obviously set up the relevant equation for H total but what will H total be equal to I guess right so let us write down H total for H+ - concentration of H0 - +HAC and that is equal to what now it is now source and that is going to equal to 0 that is the change here I guess. But with respect to AC total what you are going to see here is going to be equal to concentration of HAC at equilibrium also concentration of a state ion at equilibrium and that = 1 times concentration of NAAC naught initial that = 10 power -3.

So we can obviously solve for this so instead of solving for this let us go ahead and plug this in and let me look at my estimate of 7.2 right. So let us go ahead and plus this it so we NA total and power -3 H total is 0 estate total is 10 power -3.

(Refer Slide Time: 10:20)



So I am going to switch here and edit list I thought I have plugged it in I guess not 0.3 and the estate total is 0.001 right 0.001 and I am going to add that to the list right I am going to check the list okay and what else I need to add H total ABCDEFGH H total though I believe was added to the list and then set it to be 0 here and then total as we know was 0 right to just 0 their the jus 0 and again back to main menu and again I am going to add NA + and A I guess I miss you something here sodium right and that again for = 0.001 and I am going to add to that + new edit list 0.001 so on and so on right.

So that is what we have here and back to main menu we need to calculate the PH ionic strength is not fixed I need to calculated and the u its are molal I could have used milli molal and 1 I will do that later and so I am going to run the VMINTEQ and let us see what we have I guess I am slightly half from my particular value looks like PH here slightly higher 7.8 and let us look at what the species are did we approximate the species well enough.

So we did look at high species I guess right 1, 2, 3 ,4 and 5 so we did list NAAC and NAOH because in general they would be present at various very low concentration and guess that is what you would see here yes so NAOH is present at very low concentrations and even NAAC is present at very low concentrations so some of the take home messages are ionic strength is very low and that is why concentration and activity or more or less being the same because activity coefficient are going to be now negligible not negligible I guess their going to be = 1.

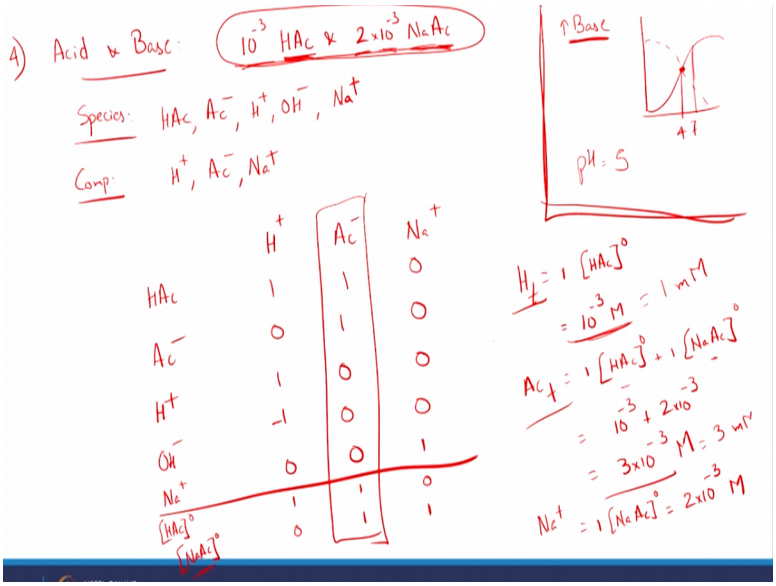
So that is what you see here and let us look at species distribution what is this give me an idea about and what form is estate present as so look like almost 100% of it almost anyway present at AC- right and that is what you see here and very little point less than 1% is present as NAAC and HAC that is what you see here right and also NA+ is present almost 100% and more than 99.9% as NA+ and very little is present as NAAC right.

So we are done with that again this is what we expect why this is estate AC- so high in concentration because PH is far greater that PKA right so that is why you see that more or less all the estate or estate total is present as AC- so again keep in mind that we have the PH versus ionization fraction right and we know when the PPH is exceeding PKA what do you expect now we expect that equilibrium at that particular PH when PH is greater than PK.

Again we are going to expect why is estate AC- so high in concentration because PH is far greater than PKA right so that is why you see that more or less all the estate or estate total is present as AC- so anyway keep in mind that we have the PH versus ionization fraction graph right and we know that when the PH is exceeding PKA what do you expect now you expect that at equilibrium at that particular PH when PH is greater than PKA again you are going to expect that the proton not proton pardon me the relevant acid is going to stain its deprotonated form.

And for the acetic acid what is the deprotonated form it is the state ion so that is what we see here right and as PH7 or in this case 7.8 I guess right that is what we need to calculate the far off from 4.7 which is the PKA of your particular acetic acid so that is why almost all of your acetic acid is present in the deprotonated form which is the estate ion I guess. So anyway estate total most of it is estate ion and take home message of 7.8 so let us go back I guess and look at the other example that I have for today.

(Refer Slide Time: 14:47)



So I am going to switch here so I am done with this particular case so we will look at the other example and I believe the other example is such that we are going to add both an acid and a base. So earlier we had only one acid or one base so this time though I see to that we are going to add an acid and base so we know that the source compound with species are 10 power -3 HAC and 2 into 10 – 3 NAC.

So you are adding an acid and you are adding base at acid concentration and from our background we know that the PKA value is 4.7 so the first aspect it is we need to do that is we need to or we are trying to intuitively guess the answer right so let us try to do that I guess so here we have we are going to try to guess that and we have relatively equal amounts we have higher concentration of the base twice right.

So we have the HAC and AC – but AC – is higher concentration so the first case that I can guess that you are adding the same type of acid and its conjugate base so the PH is going to be nearer to PKA if we had same concentration of acid and base to water. But here the PKA is 4.7 but you are adding more base so what would be there be then or what would the PH can be done it I would be slightly higher than a PKA value again if you add the same quantities of your acid and conjugate base you are going to have your particular PH nearer to PKA.

But now you are adding twice as much of your base as your acid so what I am presuming is that the particular concentration pardon me PH of your particular system is going to be higher but not

by great value when compared to your PKA so let us say why this is I guess so here not why just a basic explanation to PKA is 4.7 so we added them at equal quantities we will have them at 4.7 PH but if am adding twice that and the concentration are not too high not too low either so I am going to go with 5 may be PH5 so let us say I guess it is going to be equal to 5 why is that because I have higher concentration base compare to the acid.

So again briefly let us set up our particular system right we are going to use the species the components directly we are going to go into do the tableau today or this time anyway and then we are going to set it up in VMINTEQ and check our answer I guess right. So let us list our species so you use species you would expect our what is it now HAC and AC- and certainly H+ and PH- and then NA+.

So we are neglecting the other minus species that we came compare we believe that we came across NAOH and sodium estate 2 but as you see it is less than 0.1% of 10 power molal means they exist at little too negligible values i guess so any way HAC- at least with our acid base chemistry background we should have HAC and AC – and H+ and OC- and obviously solved NA- so let us try to write down our components what is going to change not match because there are still the same we are going to have H+ AC- ad NA+.

So these are all three components so let us directly jump on to the tableau and here I am going to have the species HAC AC- and here it is going to be 1 0 1 -1 0, 1, 1, 1, 0, 0, 0, 0, 0, 0 and 1. But the issue is that we have two source compound or recipe species they are HAC naught and NAAC naught so we have two recipe species so H+ that is going to be 1 here and again HAC1 and 0 here and again here it is going to be 0 no contribution to NAC AC is going to be 1 and NA is going to be 1.

So first we need to have our H total so for VMINTEQ what do we need to specify I guess we need to be specify the components right and the total component concentration which is what I am trying to calculate here or we are trying to calculate here right. So H total what is that equal to 1 times HAC naught and that is equal to 10 power -3 molar and what about AC total though that is equal to 1 times this what we are looking at = what do I have here HAC naught + 1 times NAAC naught.

And what are these two compounds we get that from that initially these are two compounds that we are putting in our system right. So now we have that is going to be equal to HAC naught is 10 power -3 + 2 into 10 power -3 that is = 3 into 10 power +3 so these are the two values so our two components that are going to plug in into my solution. The units are molar units here so switch so let us look at view edit list and again the sodium NA+ = 1 times NAAC naught and that is going to be equal to what naught NAC naught into 2 into 10 power -3 molar.

So I will switch now this time I will switch to milli molal units and I know that what is my particular value please and I know that sodium was equal to I believe 2 milli molal so I will say add that to the list and what else do I need to have. I need to have ahh say key disappear I guess H total = 10 power – 3 and is total = 3 times 10 power -3 so let us see if I can edit that list here H total = and again the key H total was = 1 milli milal I believe.

And estate = 3 milli molal right so this now the units were back to main menu the units where milli molal let me again just check 31 and 2 H+ is 1 and estate is 2 let us check that again please. So H total is milli molal 1 milli molal and this is equal to 1 milli molal and let us switch and check 1 and 3 right we are on the right track so everything else seems to order and run my VMINTEQ and first aspect is wellbeing we have PH.

Let us have PH as 5.042 and I believe we estimated to be around 5 or such so that was a decent guess their and then we have the relevant concentration and activities right here we have a slightly higher ionic strength what is the reason why we some deviation with respect to our activities let us still relatively dilute values and again major a or spect to look at is species distribution so NA + always going to stay as solved so NA+ itself so 99% of NA is put in stay as NA+ at equilibrium and this particular so as PH 5 right.

The PH is 5 and we know that PKA value so PH is 5 and PKA of this acetic acid is what now 0.7 so what is that mean you are going to have a slightly higher concentration of estate of deprotonated form that is still significant amount of your protonated form so let us see if you have that is what we see here. So 66% has hesitate of the deprotonated form and VC is that have the HAC or the protonated form we have 33% again the total should obviously be equal to 100% and that is what we see here and so we are done with today's class I again.

So we were today able to look at again few more examples one with respect to machine of bass and then addition of both an acid and a bass and estimated to an acid and then looking at total component balance equations to be able to calculate your what do we say PH using VMINTEQ. So with that I guess I will (()) (24:02) and we will meet in the next lecture session and thank you.