Environment Engineering: Chemical Processes

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Module No # 02
Lecture No # 06
Component Balance

Hello again welcome to the chemical process course so we are again go back to our quick review of what we discussed in our last class right.

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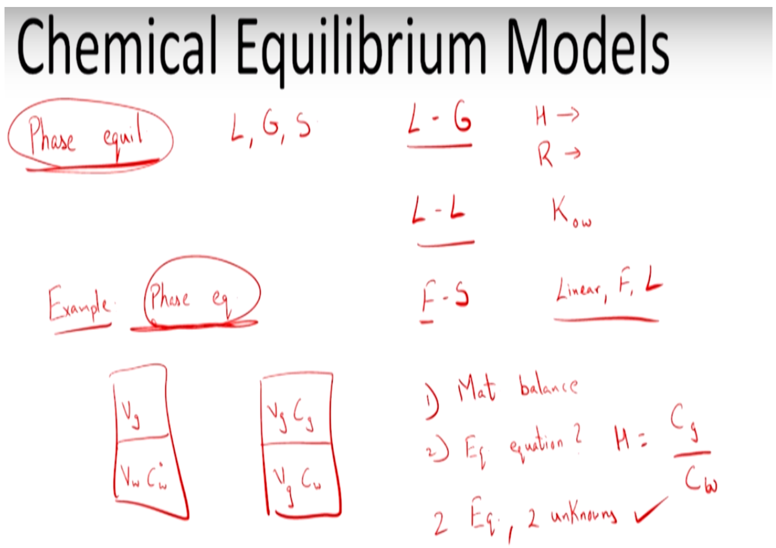

So I believe most of the time we spent looking phase equilibrium phase equilibrium and the different phases I guess what now liquid gaseous and solid phases so we looked at some of the morals give us an idea between portioning of the compound between liquid and gas I believe we looked at Henry's law and Rauolt's law. Henry's law in the dilutes systems Rauolt's law in non-dilute systems right.

And then we looked at liquid – liquid partitioning and widely used variable is the atonal water partitioning coefficient is something that we looked at and then fluid and solid fluid is either a liquid or gas right we looked at various models for this partitioning I believe we looked at linear (()) (01:23) models right and then we also looked at one particular example of phase equilibrium example of phase equilibrium.

So we have two phases or if I had two phases one is water and one is gas so we had initially all the compound only in the water and after equilibrium or phase equilibrium after phase equilibrium we wanted to calculate what is the concentration at equilibrium in both the phases right. A particular compound was initially only and liquid phase and later on and both the gaseous and the aqueous or water phases right.

So we looked at two aspects their we looked at material balance or mass balance and then because if it is phase equilibrium right we looked at relevant equilibrium in equations right and what was that I guess that is going to be we looked at Henry's law right which give us the relationship between concentration gaseous phase to the concentration in the water concentration of the relevant compound in gaseous phase to the concentration of the relevant compound in water at equilibrium.

So once we had this we had two equations for two unknowns and we can go head and solve the systems and this was with respect to the phase equilibrium and the example two was relevant to phase equilibrium and so then we moved on to chemical equilibrium right.

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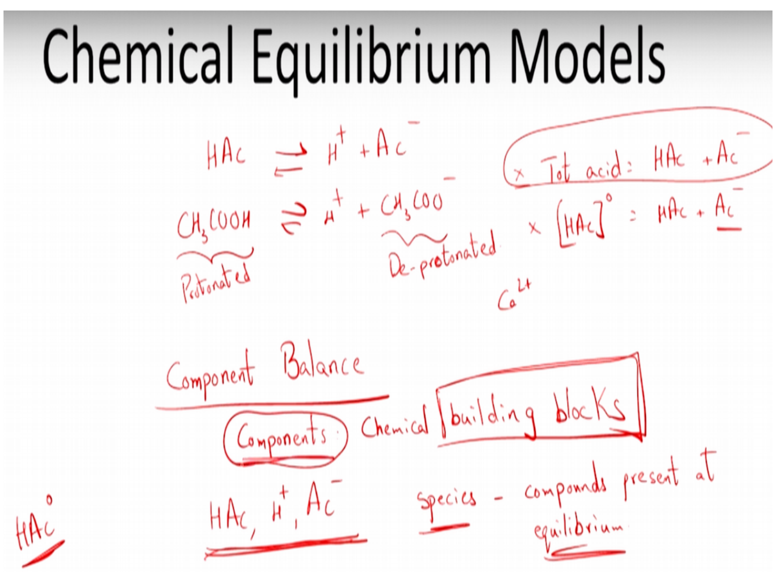

And we looked at a particular example of acetic acid and I believe I am using HAAC as representing acetic acid so it can associate into H+ and AC – right similar to not similar i guess. So how do we calculate PH the relevant concentration of the de protonated acid apart from de protonated base and protonated acid right protonated form and deprotonated.

I guess its self-explanatory right and we looked at particular simple model where we improve have a newton called total acid would be equal to HAC and AC – and we know total acid was put in initially HAC naught and we could calculate that and move ahead with our solutions now right. But the issue was if you have any other compound like calcium or any such ah matter let us say complex with your estate then this equation it is going to be invalid of this particular total acid equation is going to be invalid and we were not sure about to go forward.

For that we are looking at generic approach and that is going to be a component balance so this is something we will discussing throughout the class the component balance. So we are going to introduce a new concept here so we are going to define components here and they are nothing but chemical building blocks. So I will try to make it easy to explain in next slide but I need to give some background.

So for example I guess in this particular case let us say if it is HAC H + and AC – are the three species and again another term species compounds present at equilibrium I guess so species are those compounds which are going to present at equilibrium and in your particular solutions right.

So then we need to define something called components which are called chemical building blocks right building blocks why do they called them building blocks and in people might have certainly played with this at home I guess when they have child they have a building blocks you can use the to build different structures right. You can dismantle them and put them together to get different shapes right.

So again I think the concept is relatively symbol and that is what I get towards to get you towards I guess will come to this. So for example here the system is that initially I am putting acetic acid in the solution and I want to know the concentration of these three species here species what are they have a compound present at equilibrium in your solution right. So for this generic approach which is applicable every time I need to be able to define components.

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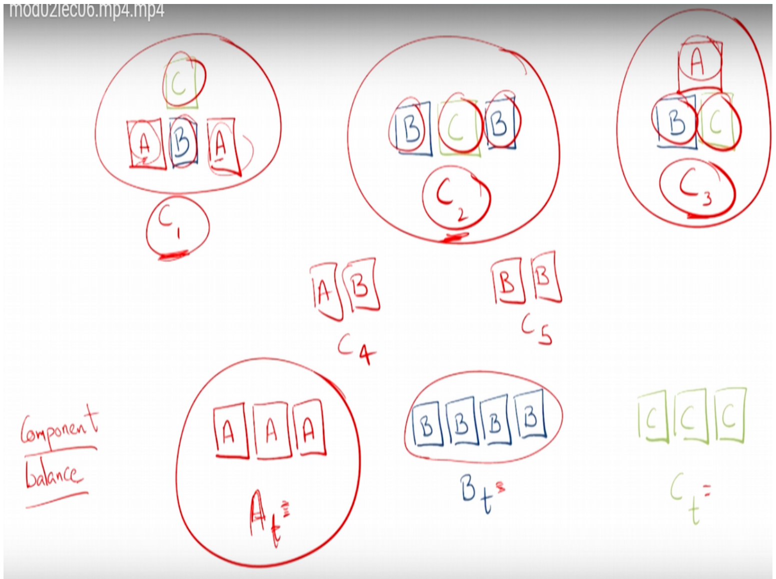

Before we go further let us look at the next slide which I have here so here let us say you know I have three compound I guess call this compound 1, Compound 2, Compound 3 I guess you know to make you understand I am using the analogy with respect to building blocks let us say right. So here you can replace these three compounds by HAC AC – or H+ or any other examples that you can think of let us say right.

So if you look at particular system not system pardon me the compound it has how many building blocks 3 has again 3 building blocks and three different kinds of building blocks there are four building blocks here but three different kinds of building blocks in C1 2 different kinds of building blocks C2 and three different kinds of building blocks in C3.

So what we are trying to look at is I am calling A right the building block A total how many is that equal to that is equal to 1,2 and 3 so that is what I have here and what we are trying to look at here is that the total number or total component is going to be conserve. So that is called the component balance right and same case here now here again I have B total and that is equal to 4 how we will look at that 1 building block here second third and fourth.

So the total building blocks with respect to B or B total = 4 here I guess right and again same case with respect to C total here it is 1, 2 and 3 yes C total again here this is what we have here. So what we are trying to get it is say I can use A and B and I guess I am using same color 10 so that going to get down faster so that please excuse me so this can be a compound 4 or B and B can be a compound 5 right.

And then the total can change depending upon the system but for one particular system the A total or B total and C total will always be constant and you know the rearrangements of these building blocks A and B within each particular compounds can change though again we are developing a concept of a component balance. So I will try to clear up hopefully in the next slide I guess right.

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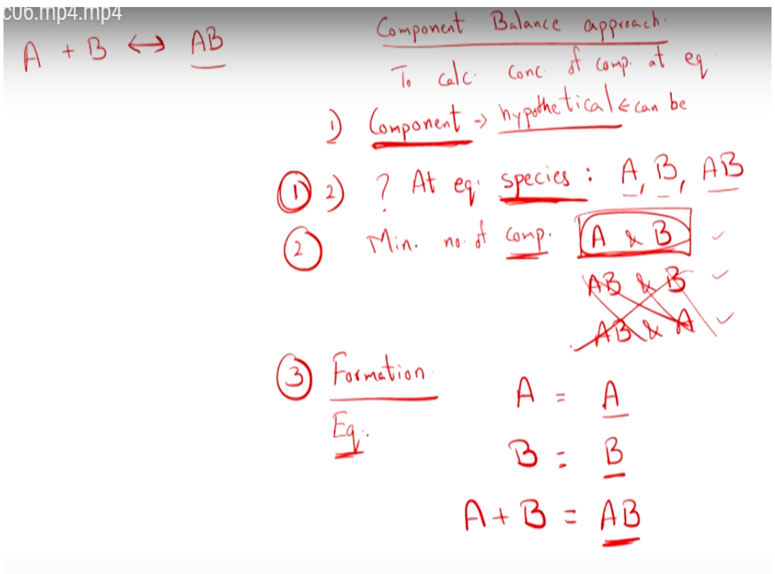

So let us look at one example here and take you through the relevant steps involved here we will consider relevant or a simple example here A + B is going to form C or A and B or hat do we say reacting it each other and forming C and this let us say reversible or you know this system can be at equilibrium. So in general in this component balance approach this is a component balance approach which is applicable everywhere are in all the situations right to calculate concentrations of compounds at equilibrium right.

Minor change to my example is going to be that instead of C obviously to make you understand I am going to call that as AB right. So compound A reacts with compound B form a new compound call AB and this will at equilibrium let us say or this can be at equilibrium. So what do we need to define I guess we need to define our components which are conservative quantities. So obviously I guess I am calling this 4 step but we will see why there is there will an issue here.

To be able to define components first need to know that is going to be present in my solution right what is that mean at equilibrium? What are the different species present? So first I need to be able to less these species not the components so first I will identify all the species present at equilibrium so what does it mean? In this case it is A, B and AB right the first step would be identifying the species.

So once identify the species and I will then choose components right minimum number of components to be able to form all my species. So when I say form though it is not a chemical reaction it can be any hypothetical equation so here what do I need to what are the components in this case I can choose A and B right or I can choose AB and B or I can choose AB and A but in general most simplest form will be the simpler building blocks we can choose A and B as my building blocks right.

So all the three forms are component what do we say forms are feasible but in general for calculations and get in the relevant constants later on easier to choose the simpler building blocks which in this case are going to be A and B right and then the next step would be writing the formation equations and one aspect here I need to clarify is that the components right the components they can be hypothetical blocks.

So they do not need to be what do we say something you would see and what we say nature or such but in general it makes they can be hypothetical can be hypothetical but species are what would actually observe or expect to see that equilibrium in the solutions right. So formation I guess so formation has an we are trying to form all the species A, B and AB how can I form them this is not a chemical reaction keep in mind.

So I need one block of A to form 1 what do we say compound A I need one block of building to be able to form one block of B and similarly I need one block A and 1 block of B to be able to form the compound AB. And the choice of the components in this case was components A and component B right we are not looking at these particular combinations yes. So these is what we have the formation equation keep in mind that these are not what do we say simple equations right.

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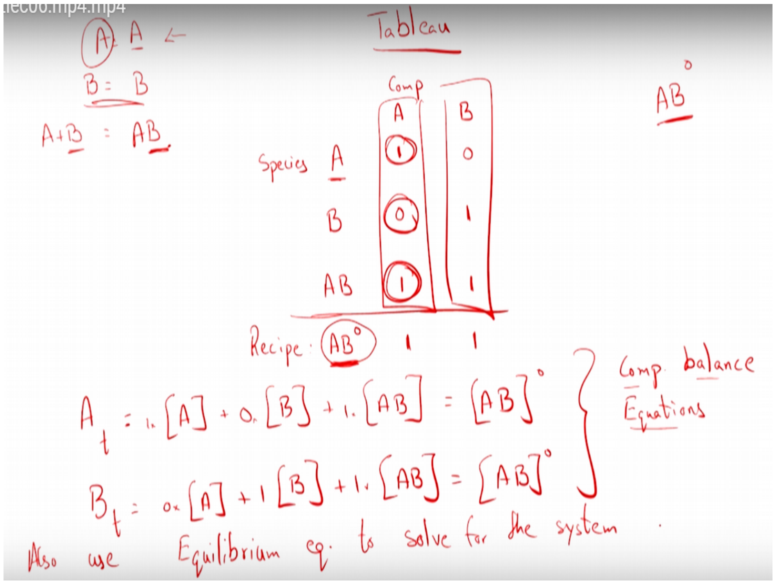

So again let us moving on then we need to I will just write this up here so then we are going to have to less the tableau right. So there we are going to have difference components and the columns and the rows are going to be species. So components in this case where A and B and the species in this case where A, B and AB and then I am going to look at the relevant what we say contribution.

So I need one component of A to be able to form species A right and 0 here and 1 here and again I need 0 of B to form A I need one of B to form B and one of B to be AB here right again let us look at that this obviously I have from your formation equations now right. The first formation equation how many A need to form A obviously one that is what we form here and one many A need to form B 0 and how many A I need to form B I have one same case with respect to B right.

And I guess we need to have the recipes species or the initial species that we are added and as you now let us say ok we will come to this with respect to the example but for the example initially we added AB naught let us say to your solution you will say that is your recipe species so that is going to be 1, 1 here I guess yes and then the component balance equation right A total = concentration of A which is this here one time concentration of A + 0 times concentration of B + 1 times of concentration of AB that is what you see here.

I am just balancing out this particular component similarly I can balance out the component B and B total is going to be 0 times concentration of A + 1 times concentration of B + 1 times concentration of AB right and as you can see here what is the source of all A and all B here it is only coming from approach it can always be used what are these equations here I guess these are the component balance equations right these are the component balance equations.

So in general obviously you would not have enough equations with adjust your components balance equations then you will look at your equilibrium equations to solve this system. So this is the generic approach here right so we are going to look at more specific example now.

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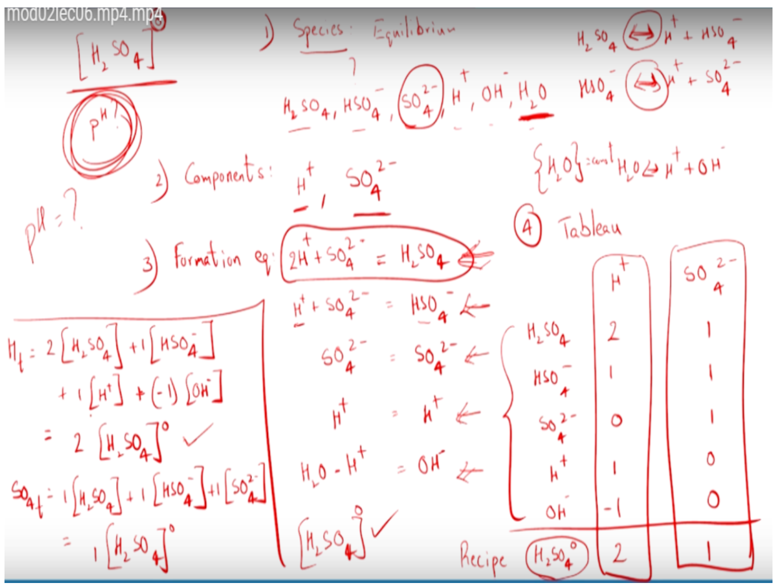

So let us say I am initially adding H2 SO4 you know of known concentration right and I want to know the final PH of the particular solution. So first what do we do here we need what do we say is the species again the example is that we initially adding H2SO4 to my system and I want to calculate the PH of this system let us say right how do I calculate the PH and in this particular term obviously or in nomenclature means + initial concentration I am adding here.

So what is our approach here species are to be listed and we know the relevant equation from acid based which will cover again the later I guess H2 SO4 is an equilibrium with H+ and HSO4 – and HSO4 – can further associate into H+ and SO4 2 – these are the two equilibrium equations or two equation that we are considering for now our when we have H_2SO_4 these are the only equation we need to consider other than obviously H^+ or H_2O dissociating into H+N and OH^-.

So this particular what do we say nomenclature means let us say at equilibrium or reversible reaction right. So what are the species here? Species are those compound will be present at equilibrium so in this case what are they so they are H_2SO_4 and HSO_4^- and SO_4^{2-} and obviously H^+ whenever we have H^+ obviously OH^- and in general if always water because these are all aqueous solutions but you know we can get by without listing water as your species because we assume that we are dilute systems and that the activity of water is more or less or constant right.

So that is why we usually do not need to list the H_2O or water as the species so now I need to choose my components and how do I do that I guess. So I want to choose these building blocks either hypothetical or real right so that I will be able to form as an mathematically I guess you can think of that form all my species right they are different combinations but most is that always be to choose as H4 as one of your components right and then look at the most deep (()) (19:16) form of pure acid base system which would then be SO_4^{2-}.

So you can use any other what do we say combinations but in general thumb rule is that to use H^+ and is to use the most departed form of your acid base system right so these are my components and the next aspect is writing the formation equations right formation equations first I will list all my what is this now species here because I am trying to form my species right and look at how I can form them.

So obviously I need two blocks of H^+ and two blocks SO_4^{2-} so keep in mind that need not be ah similar to any chemical reaction that we see this as not formation equation can be hypothetical I guess right and then we need 1 H^+ 1 SO_4^{2-} to be able to able to form SO_4^{2-} I need 1 HSO_4^{2-} to form SO^{2-} I need 1 H^+ to form H^+ and people are usually stuck with I get OH^- but if you keep in mind H_2O is always again a component H_2O or $-H^+$ will be = OH^- right.

So with this as you see I will be able to form all the five species that I wanted to H_2SO_4 HSO_4^- SO_4^{2-} + and OH^-. So here we are going to going to do the tableau right once you are proficient you can skip the formation equation and directly go to tableau right and what we are going to have here we are going to list the 2 component and what are they H+ and S04 2- and then list the species they are H2 SO4 HSO4 – SO4 2- H+ and OH – right.

And then we are going to have the recipe species we are going to talk about later so now I want to look at H+ and how many H+ we have in H2 SO4 and that is in this equation we need 2 components of H+ and many do we need them to form HSO4 – we need 1 and we need no H+ to form HO4 2- 1 to form H+ and non to form or not one pardon me going to be -1 so -1.

So they are all relevant to these formation equations here right so same case here as with respect to SO2- so how many SO2 – we require to form H2SO4 – and that is from this initial formation equation so you need 1 again same case here 1, 1, 0 and 0 yes and so as we talked about once we list the species we need to also look at the recipe species or whatever it is that you are adding initially and what is that I guess you are adding H2 SO4 initially right.

And again we need to write relevant component balance their so we need two component of H+ and one component of SO4 2 – right. So I will continue the work out here and so the total component balance for H+ or H total so H total = 2 times the concentration of H2SO4 + 1 time concentration of HSO4 - + one time the concentration of H+ - or + 1 into – 1 times concentration of OH – right and this is nothing but from the component of balance equation here (()) (23:20) and that obviously as we know = 2 times and where is this all this coming from the initial solution that we added H2SO4 naught right.

And this I what we see here and same case with respect to SO4 total and that is the balance of this particular system or column here SO4 total = 1 time H2SO4 + 1 times HSO4 – right + 1 times SO42 – and what is this all come into what is the only source of SO42- in this solution it is the H2SO4 added initially and so again 1 times H2SO4 naught. So usually what is your unknown here I guess not unknown pardon me the known H2SO4 or whatever it is that your input initially this is your known value right.

And here we are trying to calculate PH just what is the PH of the solution so if you can just solve this one equation I guess right H total will be done let us see move on the next page and how did we solve that.

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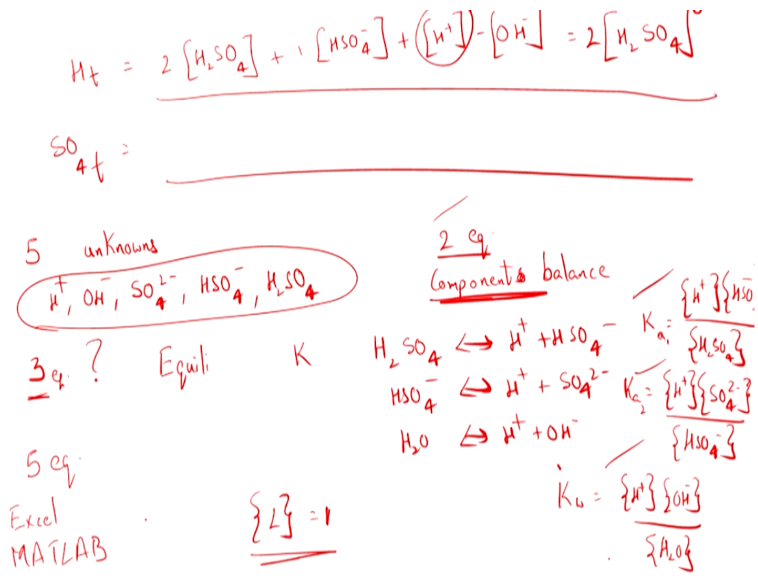

So we had H total = 2 times concentration of H2SO4 + 1 times concentration of HSO4 - + I believe H+ - OH – all these are concentration and that we know = constant called of H2SO4 that we added initially species 2 times I guess right let us see if we made any error here two times 1, 1 1 – 1 and 2 that is right here right and so here we are trying to solve this equation to be able to calculate H+ I guess right.

And so for this obviously again we have SO4 total again we have that equation but that just by two equations you cannot solve for how many unknowns how many unknowns do we have here? We have 5 species I guess 1, 2, 3 4 and 5 so we have 5 unknowns right which here what are the now H+ OH – SO4 2- HSO4- and H2 SO4 right but we have only 2 equations from the component balance so how man component balance will be equation will we have the number of component we have I guess.

So we have to component balance equations so we need three more equations independent equations so where we getting those three equations from we know the system is at equilibrium so thus we can get the relevant equilibrium constant for the three reaction we had involved what are the three reaction involved H2 SO4 can dissociate into H+ and HSO4 – can dissociate into H+ and SO42 – and water can dissociate into H+ and OH -.

So now we will have what do we say three equilibrium equations I will call this KA1 we will explain what is related and what is this equilibrium coefficient = activity of H+ into activity of

HSO4 – by activity of H2 SO4 and KA 2 will be 2 equal to activity of H+ activity of SO42 – by activity of HSO4 – and the final water dissociate I guess is going to be activity of H+ by activity of OH – and activity of H2O = 1 here liquid and here i guess activity of H2O right.

And as you know activity of liquid if it is a pure liquid again mole fraction = 1 so we do not need to list the denominator here. So now how many equations do we have we have three addition equations 1, 2 and 3 and we have two component balance equations so for the five unknowns we have 5 equations and we can solve them using excel or MATLAB right and then get the solutions ideas right. So I guess with that we will wrap up for today and look at few more what do we say examples probably in the next class before we move on to kinetics thank you.