Material and Energy Balance Computations

Prof. ARNAB ATTA
Department of Chemical Engineering
Indian Institute of Technology, Kharagpur

Lecture –22
Reactive Process Balance

Hello everyone, welcome back once again in the NPTEL online certification course on Material and Energy Balance Computation. We were in the module 5, where we are discussing the reactive processes and we started our discussion on the reactive process balance or the balance on the reactive systems.

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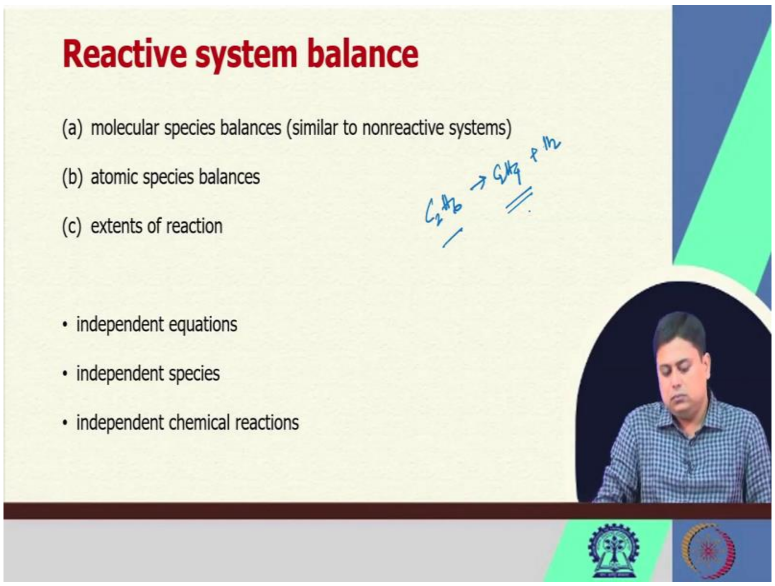

Now I mentioned last time that there are 3 ways by which we can solve a reactive system material balance and that are molecular species balance, atomic species balance and extents of reaction. So, the point is if we take a reaction say which is C_2H_6 giving $C_2H_4 + H_2$. Now say in this case we know certain amount of C_2H_6 is coming into a reactor and it is the product that is the ethylene is being formed of a known quantity.

Or say if we know that one of the product stream is known for us then how do we calculate the complete product composition. Now in that case we also consider say certain there is a known fractional conversion of ethane is happening that means in the product stream we will have some unreacted ethane ethylene and hydrogen. Now the point is you can always approach the molecular species balance and where what we have typically done for the non-reactive cases are that we take the either overall mass balance which is straight forward that is input should be output.

Except this overall balance if you apply for molecular species which are 3 here any of these 3 you need to consider whether it is consumed or it is generated. And then like the non-reactive system balance we have done it we can go ahead with the solution. One can also apply atomic species balance because in this system or in this reaction there are only 2 atomic species one is atomic carbon and atomic hydrogen.

Now as I said in the last class that this atomic species balance is quite straight forward because the atomic species can neither be created nor destroyed. So, in both the cases we have to look for input = output this scenario because this has to be conserved. So, this atomic species is relatively straight forward it in fact it is much straightforward than the molecular species balance where you need not consider whether it is being generated consumed or accumulated or etc.

It is simply you have to balance what is going in and that should come out at the atomic label. Now if there are multiple reactions you have to consider each and every reactions individual reactions and make a summation of all those as input and as output and then like we have seen in the last example the extent of reaction. Now in the first step our job always is to draw the schematic or the flow chart and then check the degree of freedom of that problem whether its 0 or not.

Now to check the degree of freedom or to do the degree of freedom analysis we need to understand couple of terms here or couple of phrases here one is the independent equation. Now you know that what is in case of an algebraic equations. The independent equations are like that you cannot derive any of the equations from the other ones either by adding or subtraction or multiplication of the equations or basically manipulating those.

So, for example you have $x + y = 5$. So, quite naturally $2x + 2y = 10$ these 2 equations are not independent you have only one independent equation here. So, similarly this independent chemical reactions is that when you have multiple reactions you have to understand or have to check whether by doing such manipulation if there are 3 reactions whether the third reaction can be achieved by multiplying say the second equation with a constant term + or – of the first equation whether that is achieved or not.

Or that such kind of manipulation exists or such kind of manipulations if that is done you land up with the one of the equations multiple equations. If that happens then definitely not all the equations are independent in that set. So, this aspect we have to evaluate before we start doing the problem or we have to identify this. Now coming to the independent species, independent species in a system when we label it we have to look into another aspect that whether this independence I mean whether 2 species are present on the flow chart with identical proportion everywhere wherever it appears or those appears together.

Say for example you have a reactor where air is being flown. Now in air say we have oxygen and nitrogen. Now this oxygen and nitrogen say is present in this ratio 3.7 times of oxygen that is the nitrogen. And throughout the flowchart it appears in the same ratio wherever it appears say either in the product stream or in the second unit when it goes out or in the recycle unit when it is recycled. It appears say in the same proportion everywhere in the flow chart.

Then these 2 species for these 2 species that is the oxygen and nitrogen you cannot really write 2 independent equations. You can write only one independent equation. So, similarly say in certain reaction this is further fed with CCl_4 that means carbon and chlorine is present in 1 : 4 ratio at the atomic label. Now if this is there everywhere this composition then it is a kind of analogous to the non-reactive species that means if the composition is not changing that is from 1 : 4 it is not changing anywhere in the system.

Then you cannot really write 2 independent atomic species balance one for Cl and other for carbon. It will be only one equation that would be independent because it is in the same proportion everywhere it appears. So, we have to be careful while doing the degree of freedom analysis because we need to be right on identifying the number of independent species that are involved in the system be it a atomic species or molecular species.

Whether the set of reactions that are given the set of reaction that is given there in the problem statement whether these are all independent chemical reactions that are happening. Because after writing the complete stoichiometric reaction you have to check whether any one of those multiple reactions, whether that can be simply a manipulation of other reactions that after writing in full stoichiometric balance.

So, based on this understanding we go step by step on the 3 methods and we have to be careful here because we will see all the approaches. But while solving any problem we can apply any one of this method because all the 3 methods would result the identical value. It must result the identical value okay the solution would not be dependent on the methods that are mentioned here that either molecular species balance or atomic species balance your overall result would not vary.

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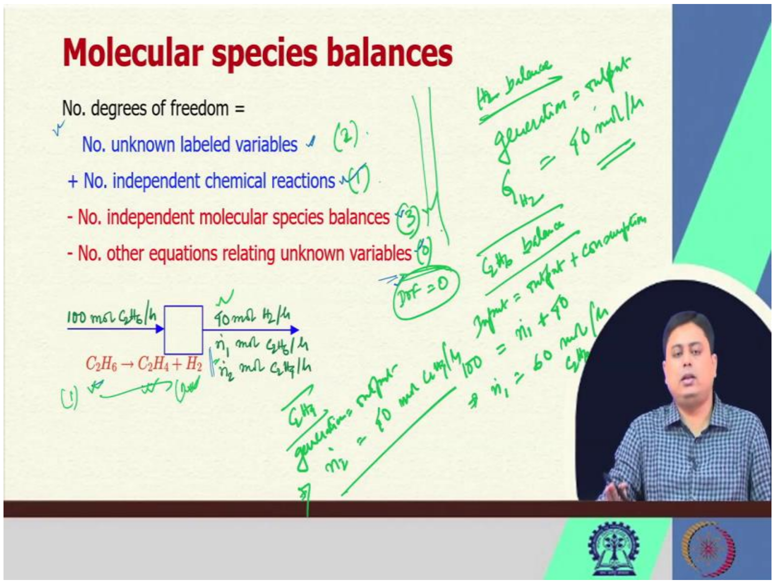

So, for molecular species balance the number of degrees of freedom = the number of labelled variables unknown variables that after understanding the problem when we make a flow chart there in that flow chart we label all the unknown variables and we count those. So, those are the number of unknown labelled variables and then we have to add the number of independent chemical reactions to that number.

Because it is now the reactions that are adding the complicacy to the non-reactive system balance because if you remember while doing the non-reactive system balance it was these 3 phrases or these 3 terms only that the number of labelled variables – number of independent molecular species or the molecular species that are involved in the system and the number of equations relating unknown variables or you can think of that the hidden information that are given in the problem statement somewhere the other.

Some physiochemical properties, the relations, some flow rate relations, some ratio of flow rates such information when it is given. So, for molecular species balance in the non-reactive cases it was those 3 terms. And here when the reactions are involved in a reactive system it adds a level of complicacy which is the number of independent chemical reactions that would be our number of degrees of freedom.

Say for example the same reactions that I was discussing we have ethane to ethylene + hydrogen say we have 100 moles of ethane coming into a reactor per hour giving the hydrogen in the output stream as 40 moles per hour. So, say our job is to find out what is $\dot{n}_1$ and $\dot{n}_2$, where $\dot{n}_1$ or n_1 stands for the ethane per hour the unreacted reactant and ethylene n_2. So, ethylene $\dot{n}_2$ moles of ethylene per hour and n_1.

So, our job is to find these 2 values. So, how do we do this or how do we at first apply the degree of freedom analysis for that or how do we perform the degree of freedom analysis. Now in this case what we have if we go by this understanding. So, how many unknowns we have in the system? we have unknowns here 2, $\dot{n}_1$ and $\dot{n}_2$ here number of independent reactions that we have only one – the number of independent molecular species balance that we can write.

In this case we can identify we have 3 molecular species. So, number of independent molecular species the balance for which we can write is 3 r 3 and number of other equations relating unknown variables no other information is given so it is zero. So, which means the degree of freedom in this case is 0, 2 + 1 – 3 that means we can solve the problem using molecular species balance and for that what should we do, we can simply write the hydrogen balance.

Now here we have to be careful when we say simple hydrogen balance because in reactive system and in this case hydrogen is there in the ethane, hydrogen is there in the ethylene, as well as hydrogen is available as the molecular species itself. So, from now onwards say we clearly mention that it is the molecular hydrogen balance, molecular hydrogen balance or H_2 balance molecular species hydrogen balance in the system.

Now in this case the hydrogen is the amount that is there in the system is purely for its generation that means we have generation of hydrogen = the output of hydrogen. So if we designate this as G H_2. So, then G stands for the generation then it becomes output = 40 mole per hour. Next we can apply C_2H_6 balance that is the ethane balance in the system. Now ethane balance is input we have certain amount that is coming in + there is no generation.

So, we cannot write anything here because it is the generic expression that i was mentioning. So, input = we have output + its consumption because in the reaction we can see it is being consumed only. So, which means here the input that we have is 100 = the output which is $\dot{n}_1$ that is the output amount + the consumption. Now how much is being consumed in the reaction we can see that for the production of one mole of H_2 we need one mole of ethane.

Here we have 40 moles of H_2 that is produced. So, that means we have consumption of 40 moles because this is the amount of hydrogen that is produced and for that we need at least 40 moles of ethane by stoichiometry. So, which means $\dot{n}_1$ = 60 mole per hour and that is specifically 60 mole of C_2H_6 per hour and then if we see C_2H_4 balance C_2H_4 there is no input it is generated.

So, generation = the output like we did for the hydrogen balance. So, we have generation = output and in this case the output is $\dot{n}_2$ and again for generating while we generate one moles of hydrogen we also generate one mole of ethylene. So, which means it is also 40 mole of C_2H_4 per hour that since we have 40 moles that is we have production of hydrogen the same amount of ethylene would also be produced.

So, I hope molecular species balance, the degree of freedom analysis is clear to you. We will apply it for multiple reactions and then the scenario would be much more clearer.

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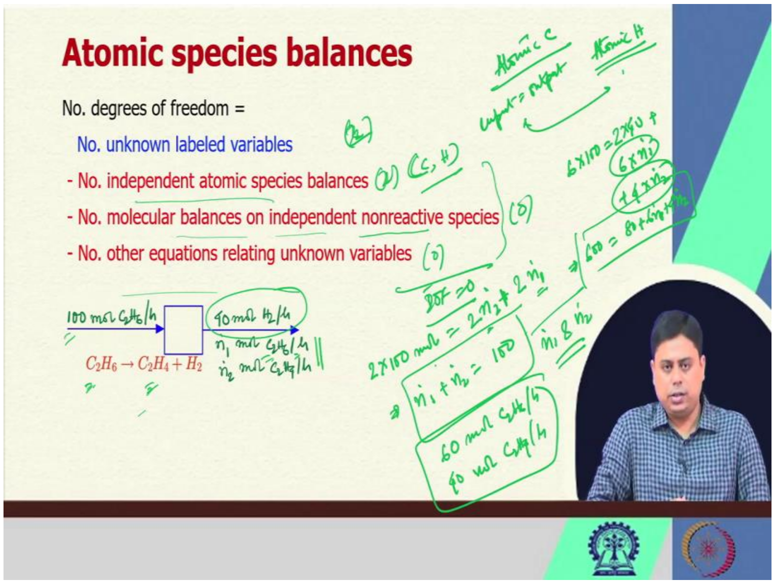

Now when we talk about atomic species balances in atomic species balance the number of degrees of freedom = the number of unknown variables that is that are labelled – the number of independent atomic species balance. And now we know what is the independent atomic species here that is the species that are not present in the flow chart or on the flow chart on a fixed proportion – the number of molecular balance of independent non-reactive species because there may be some inert in the system that are non-reactive and any other equations relating the unknown variable.

So, we have to subtract all these 3 from the number of unknown variables. So, for the same problem if we now look at it the degree of freedom in this case the number of unknown variables here we have is 2, number of independent atomic species balance that we can write is also 2 because those are C and H. The number of molecular balance that we can write for the independent non-reactive species here we do not have any such species that are non-reactive and no other information are given.

So, that means here also the degree of freedom is 0 by atomic species balance. And here the approach is much straight forward as I said because here we simply apply the atomic carbon balance and atomic hydrogen balance which is input = output in both the cases. For this case if we look at the atomic carbon balance we see the input is 2×100 mole because every mole of ethane contains 2 moles of atomic carbon.

In the output what we have is again 2 moles of carbon in each mole of ethylene. So, which means we have 2 moles of $\dot{n}_2$ + there is some unreacted ethane. So, that means $2 \times \dot{n}_1$ once again because every mole of ethane contains 2 moles of atomic carbon, every moles of ethylene contains 2 moles of atomic carbon and those 2 are the output streams here.

So, which means $\dot{n}_1 + \dot{n}_2 = 100$. So, we have got one equation and then we apply the atomic hydrogen balance. The atomic hydrogen balance again input = output and here we see that 6×100 that is the input of atomic hydrogen because 100 mol of ethane is fed to the reactor and each mole of ethane contains 6 moles of atomic hydrogen that is equals to the amount that we have is 40 rather 2×40 mole of hydrogen from this information.

Because 40 mole of hydrogen is there, hydrogen per hour is being produced and each molecular hydrogen contains 2 moles of atomic hydrogen + we have $6\ \dot{n}_1 + 4\ \dot{n}_2$ and these are coming from ethane and this is from ethylene. So which means the thing that we have here is $600 = 80 + 6\ n_1 + 4\ \dot{n}_2$. We solve these 2 equations to find out the value of $\dot{n}_1$ and $\dot{n}_2$, which would be eventually 60 mole of C_2H_6 per hour and 40 mole of C_2H_4 per hour.

If we solve these 2 equations, which is eventually the same as that of the answer that we got from the molecular species balances. So, which means irrespective of the balance approach that we apply either for molecular species or atomic spaces the answer would remain same and it has to be. So, in the next class we see the same application, same example but with the application of extent of reaction.

And we will further solve multiple reactions and we will see that the one example with multiple reactions and the 3 this balance approach how difficult is molecular balance with respect to the other balances. Till then, thank you for your attention.