Basic Principles and Calculation in Chemical engineering
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Module-11
Lecture-32
Process Degrees of Freedom

Welcome to massive open online course on basic principles and calculations in chemical engineering. In this lecture we will start to discuss about some basics of computer aided balance equations. And in this lecture mainly will be focusing on the process degrees of freedom.

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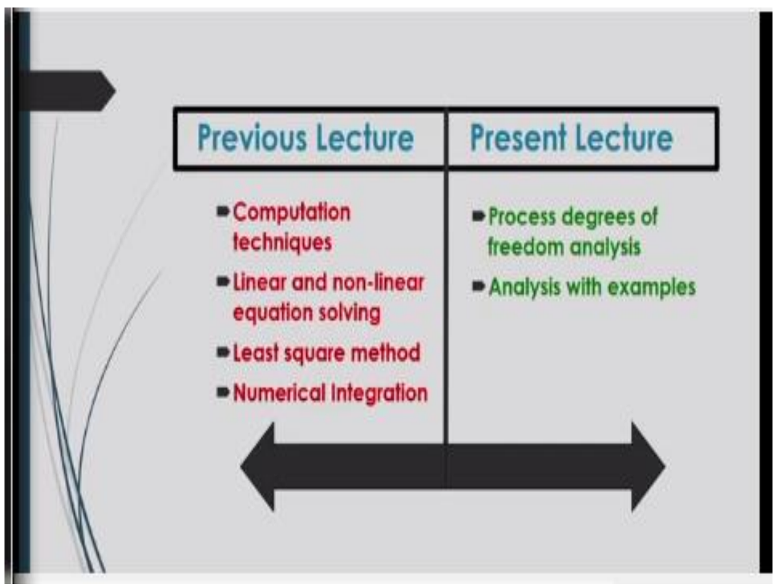

And how to analyze that process degrees of freedom with examples will be you know discussed here.

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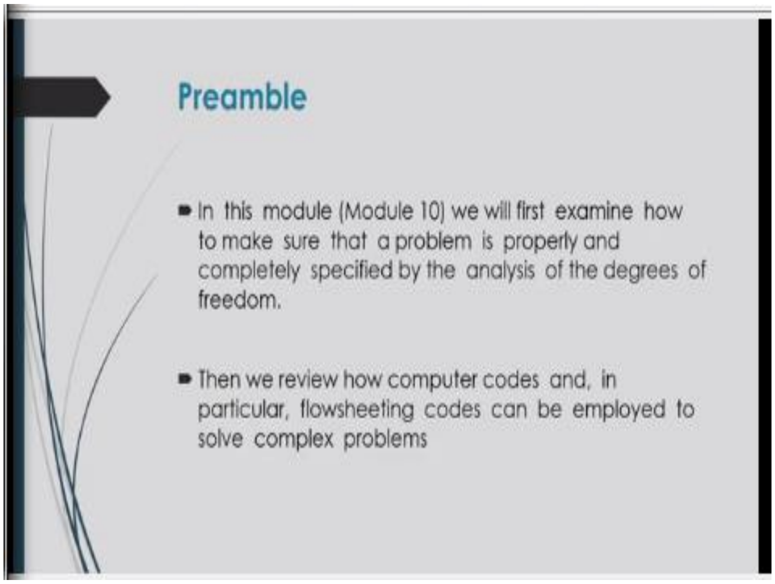

So, you know that in the previous module we have described something about the computer basics based on which how to calculate the numerical integration for a function. And also we have describe something about that least square method also we have described about solution methodology for linear and nonlinear equations. So, all those actually phenomena or you can say that topics that we have described those are computer based you know calculations.

Here also we will try to do something about some calculations, how to do the process, analysis based on modular based you know computer analysis as well as how to actually express the different codes based on the flowsheeting of the chemical engineering processes. And this will be very basic of this based on these you may be you know that able to analyze different process and how to you know handle the tools of different softwares based on this module.

Because there are various you know softwares they are actually developed based on the module based you know analysis of the chemical engineering process. And for that they have developed you know different codes based on that flowsheeting of individual units of that particular chemical engineering processes. Now based on that you know flowsheeting that is analysis of that chemical engineering process.

You have to first what should be the degrees of freedom of that you know process because it will give you the you know basis of that idea. Whether the you know solution of that chemical engineering process can be you know assessed based on that you know set of linear equation or nonlinear equation based on the material balance or energy balance equation or not.

If you know that there are n number of variables for a particular process and also you are getting that some numbers of equations that is form based on that material balance equation. Now based on that number of equations and number of variables whether these you know equations can be you know solved or unique solution or not. Or how to actually manage those equations based on that variables.

So that you can get a particular solution maybe unique solution maybe more than one solutions also there. But to get that unique solution of individual variables you have to know the degrees of freedom of that you know process. And also based on that degrees of freedom you can assess whether that equations can be solved or not. And also whether that variables to be specified for that particular process or not in that particular flowsheeting codes.

Also it may be helpful for analysis of that you know process based on that process variables whether it will be you know validated or not for that process analysis there.

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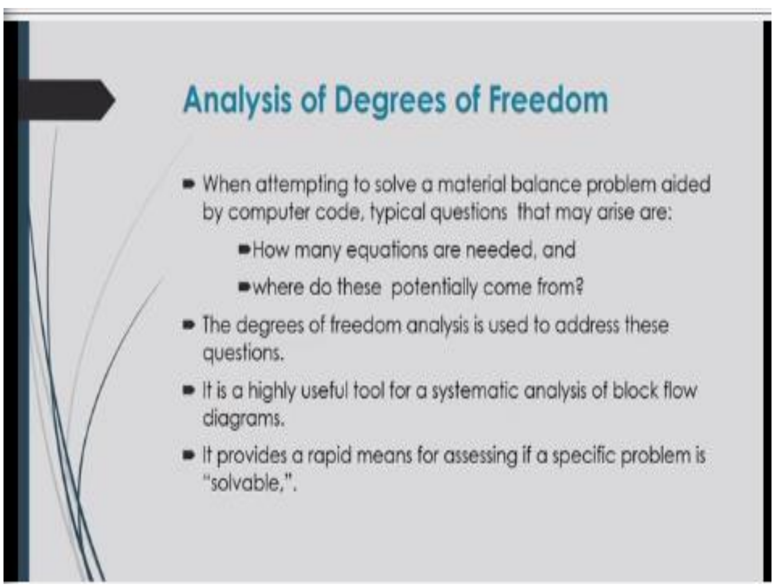

Now when attempting to solve a material balance problem that is aided by computer code you will see that typical questions that may arise. Like how many equations are needed and where do these potentially come from. The degrees of freedom analysis is used to address these questions, it is a highly useful tool for systematic analysis of block flow diagrams. And it provides rapid means of you know assessing if a specific problem is solvable or not.

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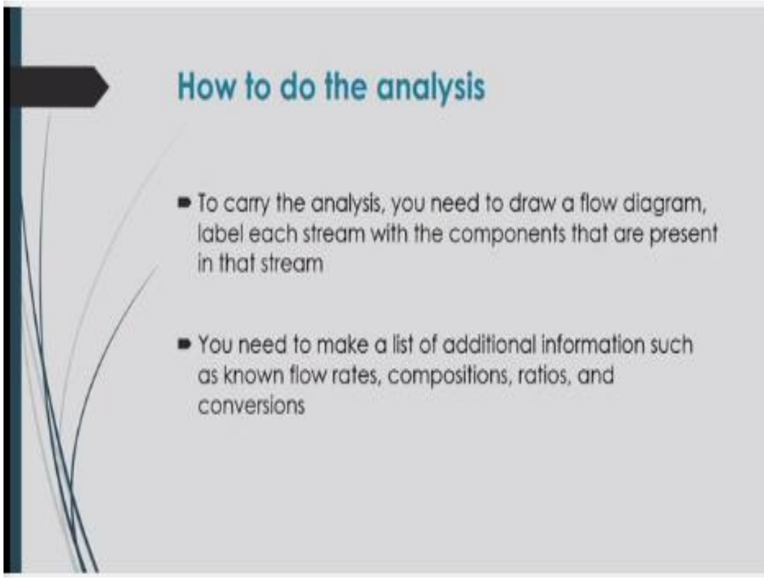

So that is why you have to know the degrees of freedom to do the process analysis. Now, to carry the analysis you need to draw a flow diagram. And also you have to label on the flow diagram for each stream with the components that are present in the stream. You need to make a list of you know additional information such as flow rates even compositions ratios. And also you can say if there any conversions or not that you have to know.

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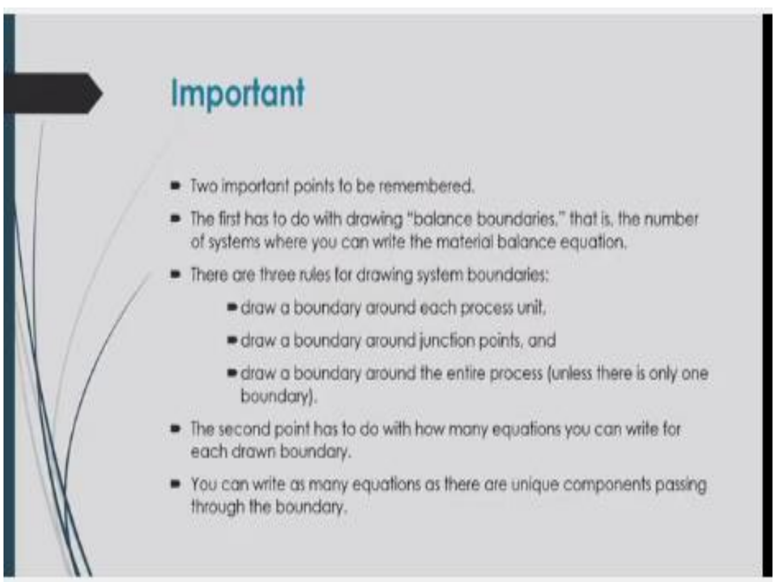

Now 2 important points that to be remembered in this case the past has to do with drawing, now balanced boundaries that is the number of systems. However you can write the material balance equation. There are 3 rules for drawing system boundaries, first of all that you have to draw the boundary around is process unit. Secondly you have to draw the boundary around junction points, and third a boundary will be drawn around the entire process unless there is only one boundary there.

It is a second point has to do with the with how many questions you can write for each drawn boundary there. And then you have to write as many as possible the equations where there are unique components passing through the boundary.

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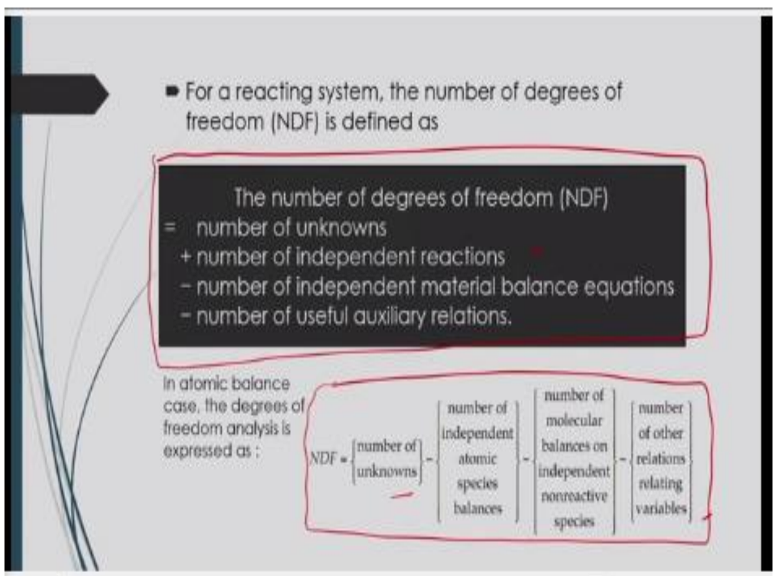

Now for a reacting system then after mentioning all those you know boundaries even processes streams specifications there. The number of degrees of freedom to be calculated based on this you know definition like here. The number of degrees of freedom that will be equal to how many numbers of unknown variables are there and number of independent reactions is happened or not there.

Number of independent material balance equations that you have to know, number of useful auxiliary relations or they are not that also you have to know. So from those number of unknowns, number of independent reactions, number of you know independent material balance equations. And also number of useful auxiliary relations you can calculate what should be the degrees of freedom for the process.

Now that number of degrees of freedom can be defined as number of unknowns plus number of independent relations minus number of independent material balance equations minus number of useful auxiliary you know relations. Now in atomic balance case the degrees of freedom analysis can be expressed as like number of unknowns minus number of independent atomic species balances minus number of molecular balances on independent non reactive species minus number of other relations relating variables.

So from these you know equations you can calculate what should be the number of degrees of freedom. And that can be you know based on the moles or that can be based on the atoms also.

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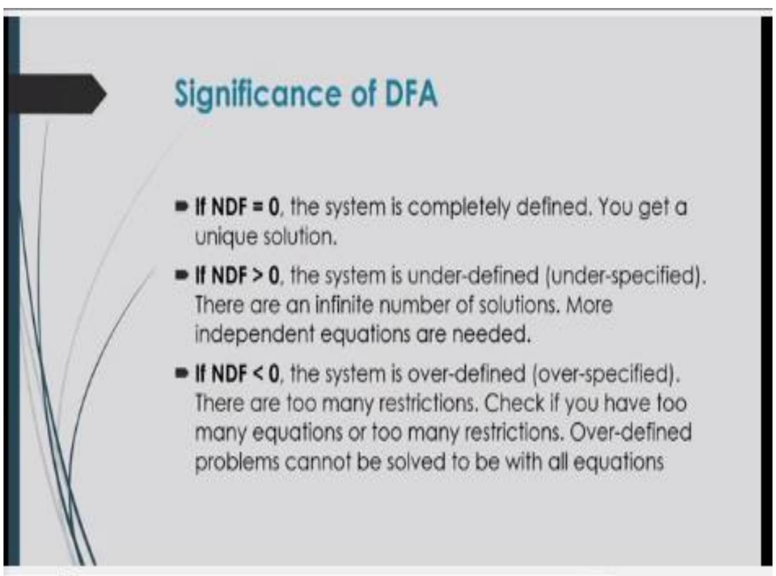

Now what is the significance of that degrees of freedom analysis, why we should do these things. Now in this case from this definition of degrees of freedom if you are getting suppose number of degrees of freedom musical to 0. In that case you can say that the system is completely defined, in that case you can get a unique solution for the system where is there any unknown variables and that unknown variables to be you know to be 1 as a solution for that particular system.

Now if number of degrees of freedom is greater than 0 what will happen. In that case, the system is under defined that means under specified. In that case there are an infinite number of solutions will be there, more independent equations for that will be needed to solve the unique solution. If number of degrees of freedom is less than 0, in that case the system will be over specified, there are too many actually restrictions will be there.

Now in that case you have to check whether you have too many questions or too many restrictions are there or not. Over-defined problems cannot be solved to be with all the equations there. So, you have to select some equations which will be equals to the number of unknown variables. So if there are over specified you can neglect some equation, if it is under specified or under defined then you have to add some other independent equations to get it is unique solution.

Now, if NDF is equal to that means number of degrees of freedom equals to 0 then system will be completely defined, there is no more equations required even no more you know unknown variables will be considered there. So like this in this way we can you know say whether the system is you know well defined or not whether it is over specified or under specified, if it is under specified what to do and if it is over specified what to do, so based on which we have to solve the problem.

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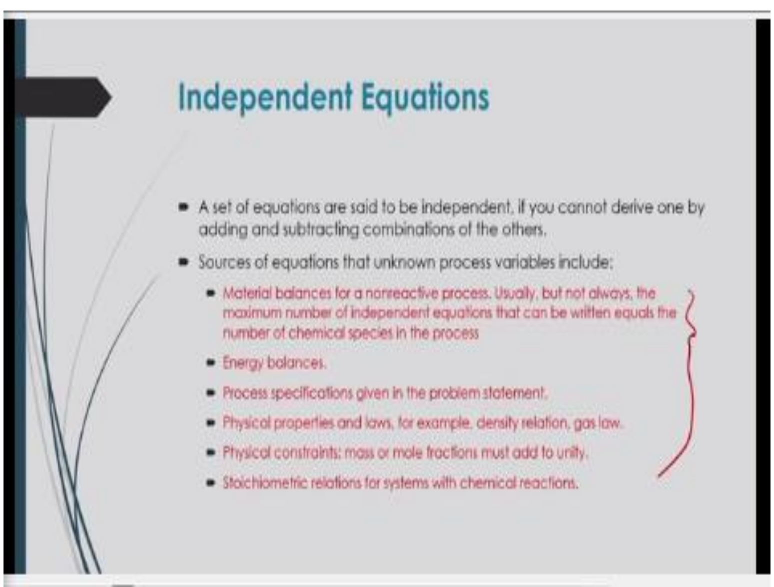

Now to calculate that number of degrees of freedom you need to have some independent equations, that independent equations to be formed based on that material balance equation or energy balance equation. Now when it will be called that independent equation, a set of equations are said to be independent if you cannot derive one or by adding and subtracting combinations of the others, so that equations will be called as independent equations.

Now sources of equations that unknown process variables include, now these equations whatever independent equations to be formed that may come from material balance for reactive and nonreactive processes. And that equations may come from energy balances, that equation may come from processes specifications, that is given in the problem statement. That equation may comes from physical properties and laws like you know density relations, gas laws like pressure vapor pressure relation with the you know composition of the you know materials in the liquid or gas.

Physical constraints, like you know that summation of more fractions or mass fractions of the you know compound should be equals to one. And then what is that stoichiometric relations for the systems with chemical you know reactions. So these are the source of generating of those independent equations based on which you have to calculate what should be the number of degrees of freedom.

And based on which you have to assess whether the system is well defined or under defined or you know over defined or not. And accordingly you have to solve for unique solution of those system.

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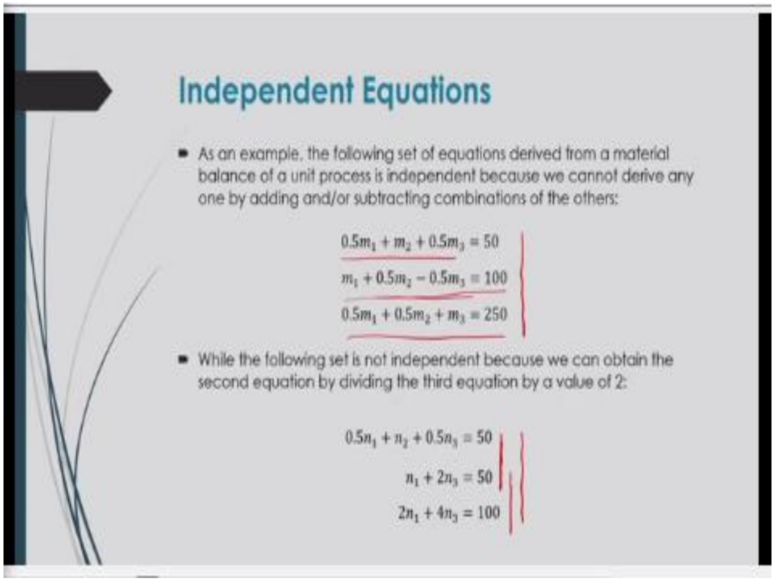

Now for independent equations let us have this the following set of equations here given in the slide, that is derived from a material balance of unit process. Which is independent because we cannot derive anyone by adding or subtracting combinations of the others. Like here you will see that these equations 0.5 m 1 + m 2 + 0.5 m 3 that will because 250. Here m 1, m 2, m 3 are the you know that streams amount whether it is income or incoming or out coming that accordingly it will be coming that material balance will give you this equation.

Similarly the second equation also based on that input or output amounts that equation can be formed similarly third equations. Now if you look at these 3 equations you will see that no equations are dependent, no equations is dependent on others. Like you cannot generate the second equation from the first one or first one cannot be generated from the second one or third one like this.

So all these equations are independent to each other, while if you look at these second set of equations you will see that there also there are 3 equations. And in this case you will see that the third equations can be generated from the second equation. If you multiply the second equation by 2 you will see that third equation will be generated. So in this case you cannot say this set of equations are independent to each other.

Only these 2 equations first equations are independent whereas the third and second equations are not independent. So you have to you know be careful for generating that independent equations based on material balance equation. And for calculating degrees of freedom you have to be very careful whether those equations formed are independent or not, only independent equations to be counted to calculate the degrees of freedom.

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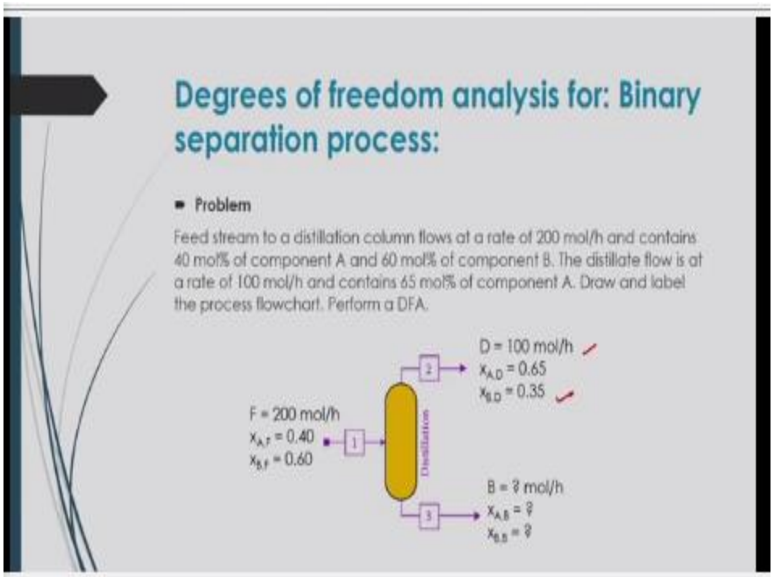

Now let us have an examples to calculate the degrees of freedom for binary separation process. Now, let us have this problem like if you have the feed stream to a distillation column that flows at rate of 200 mole per hour and contains 40 mole percent of component A and 60 mole percent of component B. The distillate flow is at a rate of 400 mole per hour and contains 65 mole percent of component A and remaining is 35% of component B.

Now in this case you have to draw the label of this you know our process flowchart you have to you know also perform the degree of freedom analysis.

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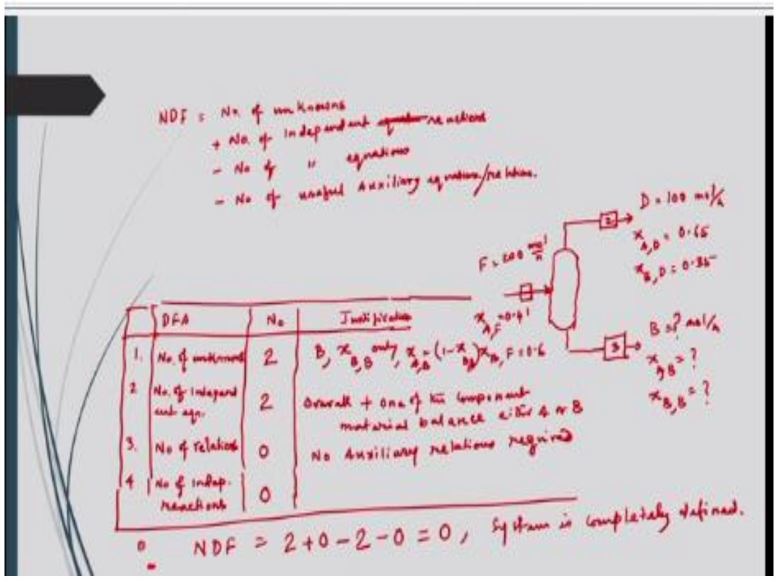

Now let us solve this problem to calculate this degrees of freedom what is that. We knew that degrees of freedom NDF, that is we calls to number of unknowns plus number of independent equations minus this is sorry number of independent here reactions here reactions minus number of independent equations then minus number of useful auxiliary equations or relations.

Now for this what to do, first of all we have to draw an label the process flowchart, what is that. This process flowchart is one is distillation column and there will be input and this distillation column through streams one let it be here through streams one. And in this case feed is given to you that is 200 mole per hour and mole fraction of components A in this feed it is given 0.4 whereas mole fraction of B in this feed stream it is given 0.6.

And from this separation by this distillation column we are getting from this stream to we are getting distillate, it is amount is 100 mole per hour. And mole fraction of component A in this distillate it is given 0.65 and mole fraction of component B in this distillate it is given 0.35. Whereas from this bottom part of this distillation column as is extreme 3 it will be coming out with a bottom amount that is unknown to you that is let it be B, this is in mole per hour.

Whereas this component A, in this bottom product B that is also unknown to you and then component B in this bottom product also unknown to you. Now based on this problem we have to calculate what should be the degrees of freedom. Let us have this in tabular format like this, it is here number of degrees of freedom analysis here number and here let it be ok justification like this.

Now if you consider here like as a serial number suppose 1 number of unknowns here what will be the number of unknowns here. It will be like 2, because here one is bottom product it is unknown to you and the composition x B at bottom product, x B only here. Because if you know the x sorry this is x, x B then you can obtain what will be the x A B.

Or if you know that x A, B here will be able to know what should be the x B B. So, in that case x A B will be equal to 1 - x B B, so by this. Similarly what should be the number of independent equations how many number of independent equations can be formed here. Here it will be 2 because one will be overall and another will be one of the component material balance either A or B.

And then you have to calculate number of relations here number of relations I think it is not required. Because there it is not suppose any equilibrium conditions or any density or any you know viscosity relations it is not required at all. So, in that case it will be 0, no auxiliary relations are required here. And then number 4 what will be the number of independent reactions, here there is no reaction, so you can write it will be 0.

Therefore number of degrees of freedom will be is equal to as per that definition. So number of unknowns is 2, number of independent reactions is 0 minus number of independent equations is 2 and then minus number of relations is 0, so it will be coming as finally 0. That means here number of degrees of freedom it is 0, what does it mean, the system is well defined you can get the unique solution of this problem. So, since NDF is equal to 0 system is completely defined like in this way we can analyze what should be the process degrees of freedom ok.

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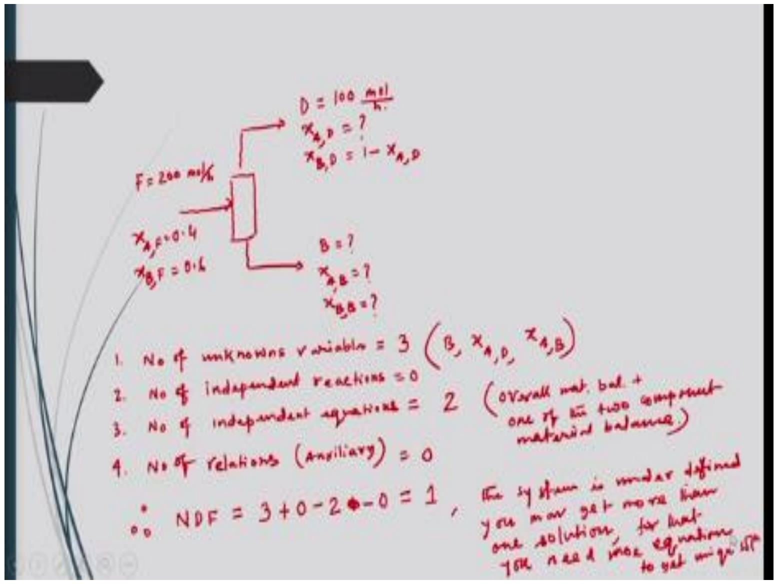

Let us do another examples, suppose a problem let us have this problem here again one distillation column. Where in this distillation column the feed will be entering at a rate of 200 mole per hour where composition at this feed as x A F that will be close to 0.4. And x B component B in this feed is equal to 0.6 and bottom product here B is unknown to you x A at this B it is also unknown to you, x B B it is unknown to you.

Whereas from this top product as a distillate you can say that distillate amount is known to you as 100 mole per hour. And it is composition here for component A in this distillate is unknown to you. Whereas in the previous example we have given that is known to you, in this case it is unknown to you and also x B D is also unknown to you. But you can find it out from this unknown variables of x A D as 1 minus x A D.

Now in this case you will see how many you know unknown variables will be there, how many unknown equations can be formed that can be also calculated. Now let us do all those things here. First of all what is the number of unknowns variables, this is basically 3 because here one is B another is x A you know that D another is x A B this 3 unknowns are there.

Number 2, number of independent reactions that is 0, because there is no reactions taking place in this separation process. Number 3, number of independent equations that will be is equal to 2. Again you can do this material balance one is for overall material balance plus one of the two component material balance. And then what will be the number of relations, is there any auxiliary relations or not, that will be equals to 0.

Because here it is not required to consider any you know relations between you know that variables like it is a temperature dependent or viscosity dependent or something is there or not, so it is not required. So, you can write here at 0, therefore as per definition of number of degrees of freedom NDF, that will be equals to here number of unknowns is 3 plus number of reactions is 0 minus number of independent equations is 2 and plus sorry minus number of auxiliary relations is 0.

So finally we are getting here number of degrees of freedom is 1. In this case, since number of degrees of freedom is greater than 1, we can say that what is the discussion that we have given here.

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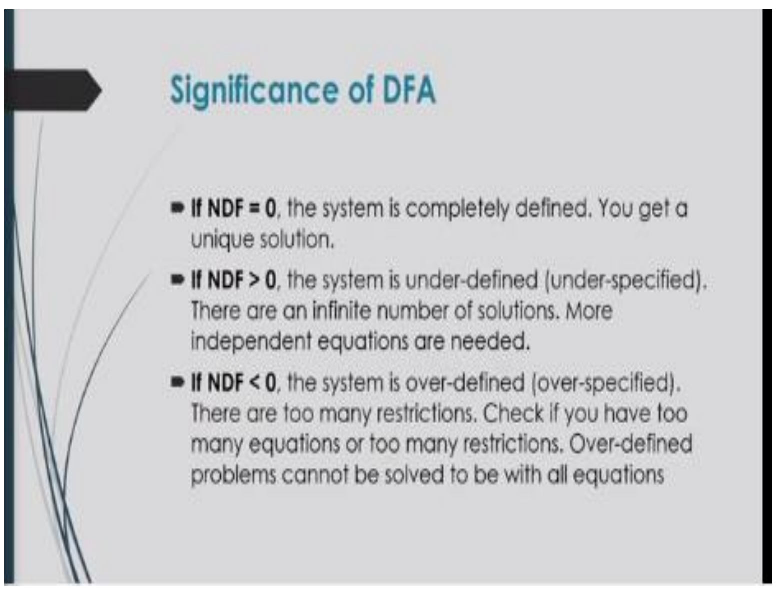

If number of degrees of freedom is greater than 0, the system is under defined, that means under specified, there are an infinite number of solutions. In that case you know that more independent equations are needed. So for this we can say this is under defined, the system is under defined, you may get more than one solution. So for that you need more equations to get unique solution.

So in this way we can solve this type of problem for number of degrees of freedom analysis. Now let us have another examples with multi component separation process, degrees of freedom with multi component separation process.

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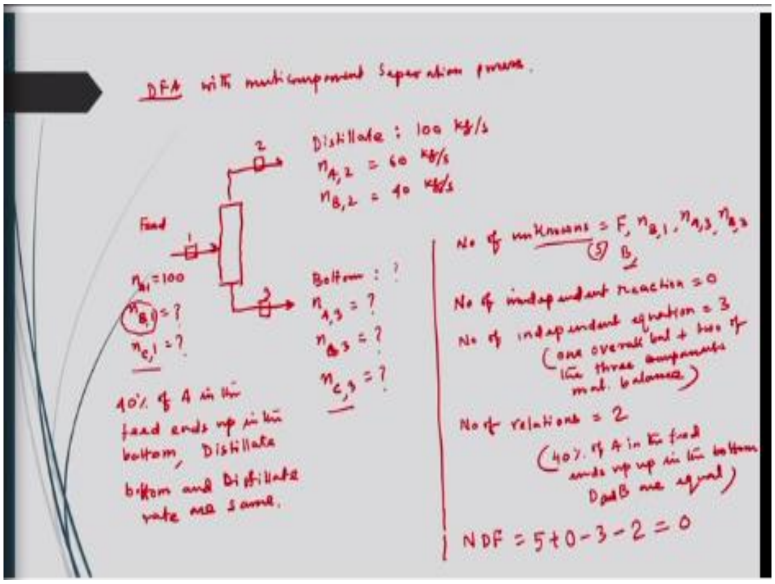

Let us considered this here, degrees of freedom with multi component separation process**.** In this case again let us consider that distillation column for your separation process your one input, there will be 2 outputs for this. In the input there will be a feed there will be a you know that moles of you know stream here let it be 1 stream 2, here stream 3.

So n A 1 means component A in stream 1, so here number of moles of component A here it is given instead of mole fractions let it be 100 and n B 1 that will be unknown to you, n C here 1 that will be unknown. Here 3 components are there that is why you are considering that here multi component separation process. Three components are there, A, B, C components are there. Now in stream 1 this 3 components are there but the amount of only one components A is given to you, others are unknown to you.

And from the stream 2 as a distillate, let it be distillate here, distillate is given here 100 kg per second. And n A 2 is given 60 kg per second and n B 2 is given 40 kg per second, and in the stream 3 here it is you know bottom product, it is not given to you. But here component wise it is given as moles of A in this 3 it is also not given to you, it is unknown n B 3 that is unknown to you, n C 3 that is also unknown to you.

So, total here B is unknown, bottom product is total, the unknown even what will be the amount of this component also unknown to you. Now in this case you have to consider that 40% of component A in the feed ends up in the bottom, distillate also will have this 40% of that, that means here 40% of A in the feed. So you can say that bottom and distillate rate are same.

So, based on which we can say that number of unknowns are here one is A, another is n B here in 1, another is n A in 3, another is n B in 3 and also you do not know what will be the amount of B there. So from this we can say that these are unknown but other unknowns like here n C 3. But you can obtain these unknown n C 3 from these 2 unknowns of this n B 1 and n B 3 if you know the total amount of bottom B from that stream 3.

So, we should not consider that n C 3 here based on because that others are known to you. And also you are considered that in the stream 1 that n B 1 is only unknown to you why m C 1 is not unknown to you. Because if it is unknown here n B 1 then you can obtain this n C 1 from this any n A 1 and n B 1 because n A 1 is already known to you. So from this you can easily calculate from the total amount of feed what should the n C 1, so we have not to consider this n C 1 here also.

And then what should be the number of independent reaction that will be equals to 0 because here there is no reaction taken place. And the number of independent equation can be formed from the material balance that will be equals to here 3. Because it will be one overall balance + 2 of the 3 components material balance. And then what should be the number of relations, this will be equals to 2, why.

Because one is given as 40% of A in the feed ends up in the bottom comma D comma B sorry in the bottom and D and B are equal. So, from these 2 relations you can say that there will be a number of relations will be equals to 2. Now we know that number of unknown variables are here that is F, n B 1, n A 3, n B 3 and B total is here 5, so total unknowns 5. Now from these you know data who can calculate what should the NDF.

So here NDF would be equals to number of unknown is 5, number of reactions is 0 minus number of independent equations is 3 minus number of relations is 2, so it will be equals to 0. So, here also you can say that with this multi component separation process, we can calculate the number of degrees of freedom. Based on this flowchart flow diagram and flowsheeting we can say that the number of degrees of freedom will be equals to 0. And hence we can say the system is well defined to get it is solution.

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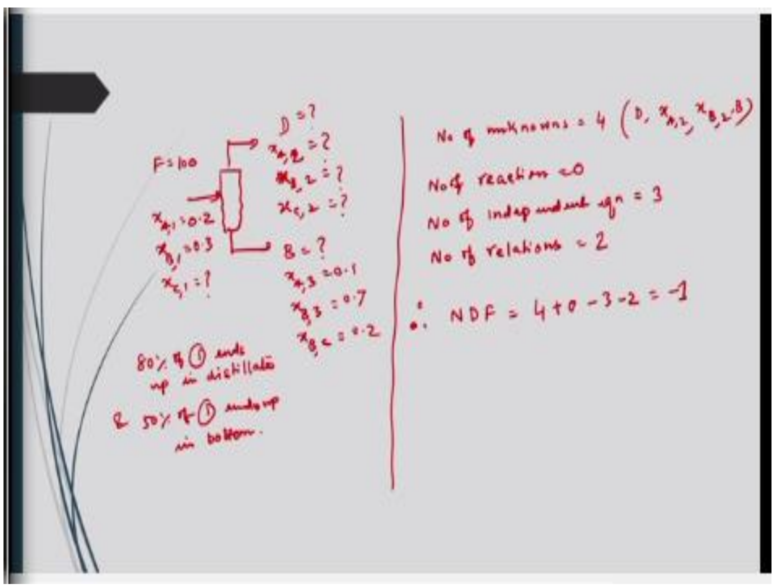

Let us consider another examples as per this diagram here like this in this case like one separation process by distillation here. Here again distillate here x A 2 is unknown to you x B 2 is unknown to you, x C 2 is unknown to you whereas here in the bottom it is also unknown to you. And then what is that x A 3 = 0.1, x B 3 that will be equal to 0.7 and x B C that will be equals to 0.2.

Whereas in the feed F is given to you 100 and x A 1 it is 0.2, x B 1 it is 0.3 and x C 1 it is unknown to you. And one important relation is given here like this 80% of stream 1 ends up in distillate and 50% of stream 1 or feed you can say that feed ends up in bottom. So based on this what should be the degrees of freedom. So in this case again we can say that number of unknowns = 4, why one is D, one is x A 2, one is x B 2 another is B and then number of reaction = 0, number of independent equation is equal to here it will be 3.

Because 1 is for overall and others, 2 will be from 2 of the 3 components. And the number of relations = 2 here as per problem therefore NDF number of degrees of freedom will be equals to here 4 + 0 – 3 here – 2 that will be equals to – 1. Here it is you know that again it is less than 0 what does it mean, that system is not well defined you cannot get the you know unique solution for this system.

So it is you know over specified since the number of spaces number of you know unknowns of the information given is more than you know the number of you know unknowns also. So we cannot this problem and for that you need to get the either you know reduce that equations or you can consider the other unknowns there to solve this equation and also to get to the unique solution for the system ok.

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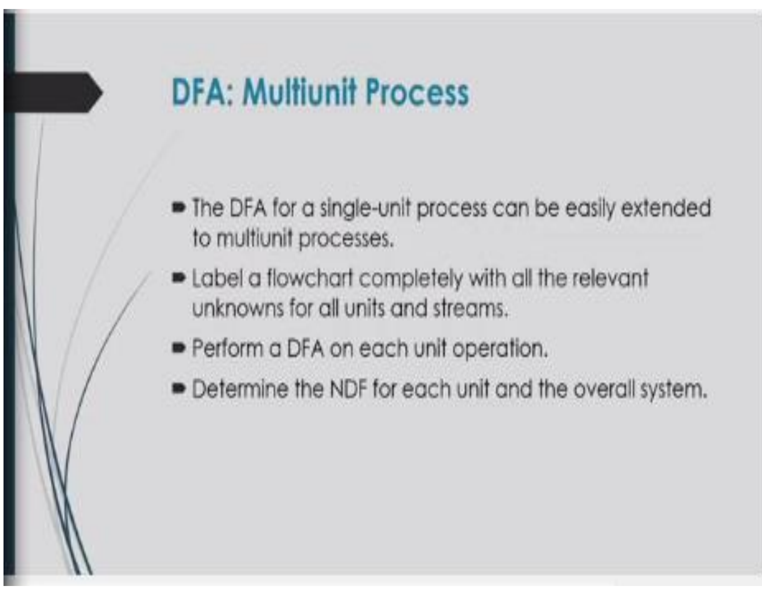

Let us analyze the degrees of freedom for multi unit processes. Now in this case the degrees of freedom whatever we have described for a single unit process can be easily extended it to multi unit process also. In that case also you have to label a flowchart completely with all the relevant unknowns for all units and streams. And then perform the degrees of freedom on each unit separately for that unit operations. And also accordingly you have to calculate what should be the number of degrees of freedom.

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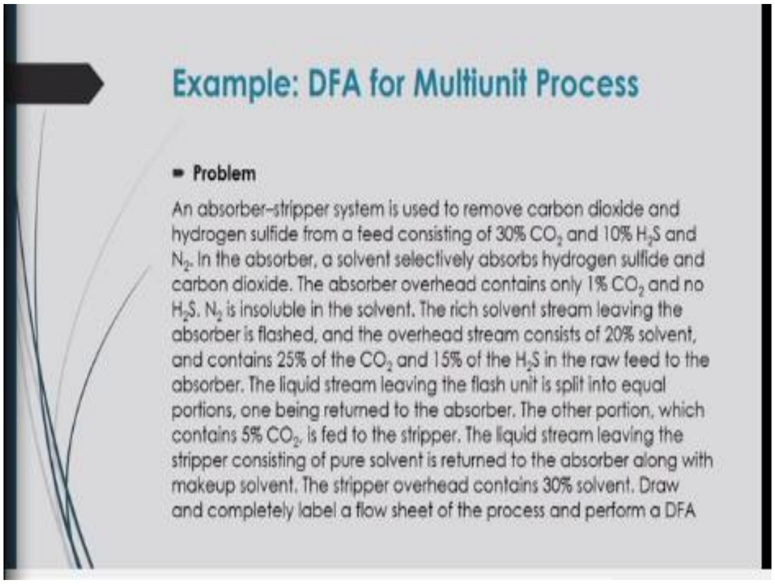

Now, let us do an example like this here an absorber stripper system which is used to remove carbon dioxide and hydrogen sulfide from a feed that consists of 30% carbon dioxide and 10% hydrogen sulfide and also nitrogen. In the absorber a solvent selectively absorbs hydrogen sulfide, carbon dioxide, the absorber overhead contains only 1% carbon dioxide and no hydrogen sulfide is there and nitrogen is insoluble in the solvent.

The rich solvent is streams leaving the absorber is flashed and the overhead stream consists of 20% solvent and contains 25% of the carbon dioxide and 15% of the hydrogen sulfide in the raw feed to the absorber. Now based on this you know problem draw and completely label a flowchart of the process and perform the degrees of freedom.

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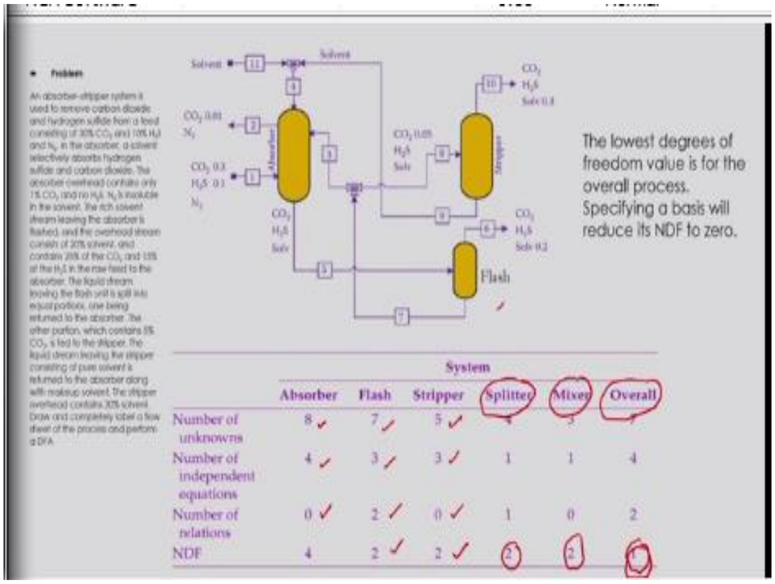

Now, let us have this you know problem with the flowchart like this here shown. Here absorber, stripper and flash units are given for whole you know process. And in the absorber here C some input will be coming an output also will be there. And there will be a some recycle from the flash and it will be send to the absorber and some portion will be again send to the stripper. And the flowchart you will see that all you know knowns and unknowns variables are mentioned there, now you have to you know perform the degrees of freedom.

Now see this number of unknowns if you consider individual you know equipment. Like if we consider here absorber number of unknowns will be 8, number of independent equations will be 4, number of relations will be 0, so in that case degrees of freedom will be equals to four. Similarly if you consider that flash you know that unknowns are there, so number of unknowns will be here 7, number of independent equations will be 3, number of relations will be 2 and then number of degrees accordingly it will be 2.

Number of unknown you know variables will be for stripper as 5, number of independent equations for stripper it will be 3 and there is no relations given for stripper. And then accordingly number of degrees of freedom will be there. Similarly you can calculate the number of degrees of freedom for stripper splitter, number of degrees of freedom for mixer, number of degrees of freedom for overall you know system.

So, in this case the lowest degrees of freedom first you have to find out and it is coming is for overall processes it is coming as 1. So which specifies that a basis will be reduce it is number of degrees of freedom to 0. So you have to you know control the system, you have to manipulate the system with some relations or variables or independent equations making from the material balance considering other you know unit.

However you will see that the last degrees of freedom will be converting to 0 there. And then you can say that the whole systems will be well defined and accordingly the number of degrees of freedom for the overall system will be equals to 0. And then accordingly we have to solve the problem and you would can get the number of you know degrees of freedom will be equals to 0 and unique solution.

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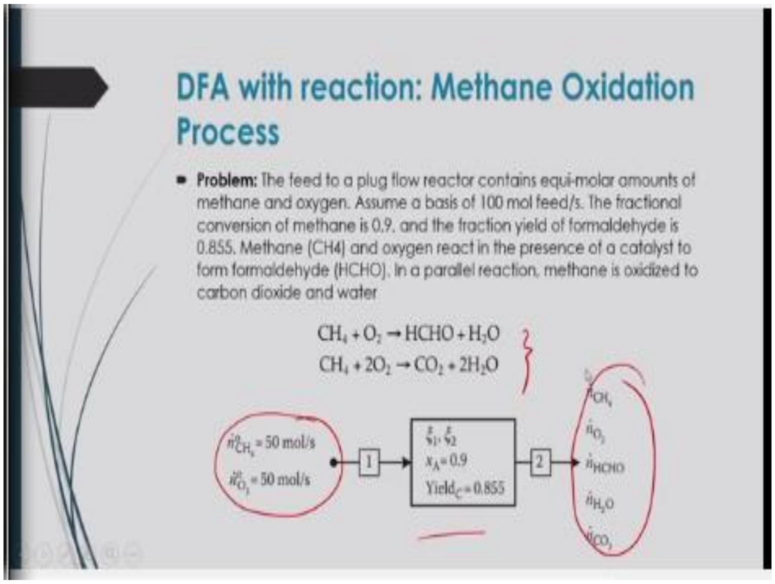

Like here if we consider another examples with reaction what will be the degrees of freedom like methane oxidation process. In this case the feed to a plug flow reactor contains equi molar amounts of methane and oxygen. Assume a basis of 100 moles feeds per second, the fractional conversion of methane is 0.1 and the fractional yield of formaldehyde is 0.855, methane and oxygen react in the presence of a catalyst form this formaldehyde.

In a parallel reaction methane is oxidized to carbon dioxide. So, here we are getting these equations and the system is specified to it is known variables and unknown variables with the streams.

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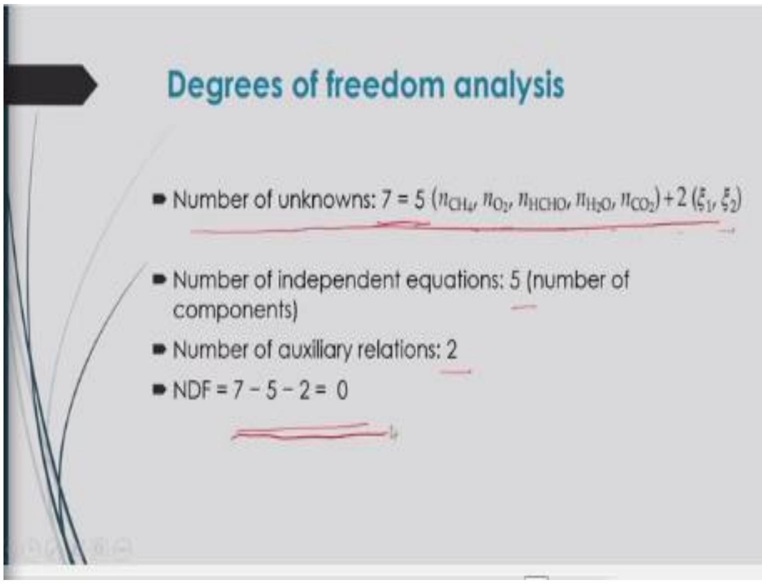

So in this case number of unknowns will be close to 7, one is methane moles, one is oxygen moles, one is formaldehyde and water and carbon dioxide moles like this and + 2 here unknowns for you know extent of reactions for this 2 reaction. So total unknown variables are 7 and number of independent equations are here that is number of your components, that would be equals to here 5 and then number of auxiliary relations is given 2, so number of degrees of freedom will be equals to 0 accordingly.

Here number of unknowns variables as per that equations here, we can say the number of unknowns is you know 5 and then number of reactions will be equals to 2. So, according to we have taken this number of unknowns will be equal to 7 + 2. So, here accordingly that number of degrees of freedom will be equals to 0.

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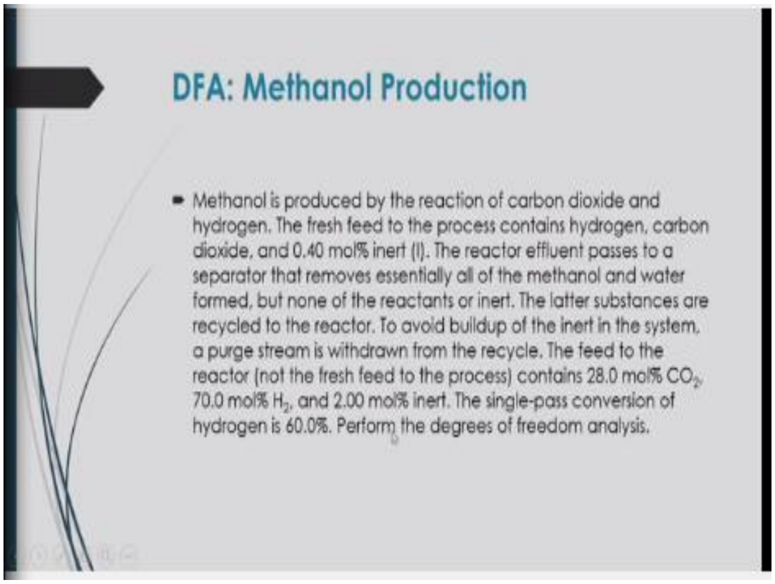

Similarly another problem here methane production.

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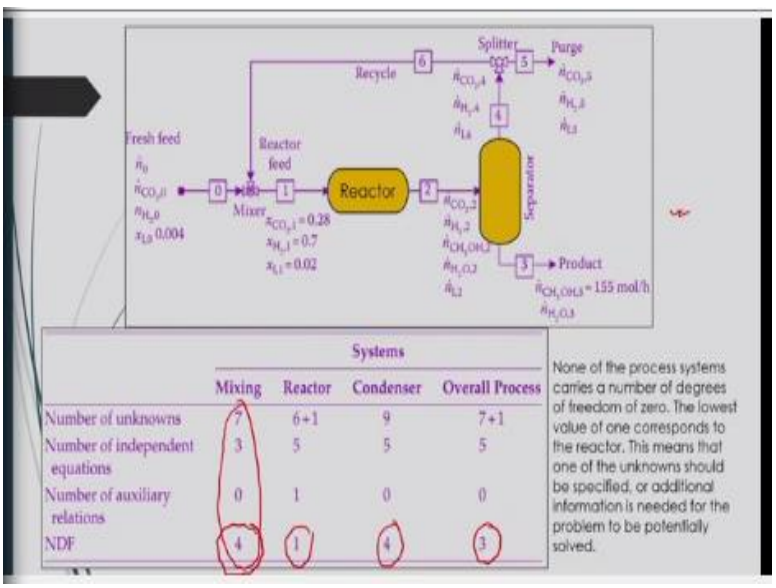

Here this flowchart is given and in different you know inlet and outlet streams for different you know units there all knowns and unknowns variables are specified. And accordingly what will be the number of unknowns, number of independent equations and number of auxiliary relations are given. And then according to what should be the number of degrees of freedom that is analyzed based on individual equipment, it is shown in the slides.

And then we can say that none of the process systems here carries, in number of degrees of freedom of 0 here. And then lowest values of 1 corresponds to the reactor here, that is 1 and this means that the one of the unknown should be specified here and or additional information to be needed for the problems to be you know potentially solved. So, in this way you can analyze the degrees of freedom.

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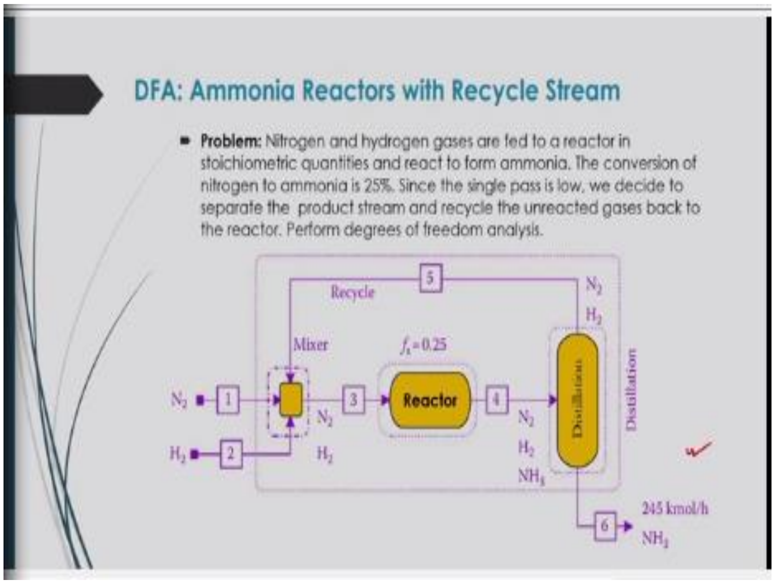

Similarly another example is given for ammonia reactions with recycle stream.

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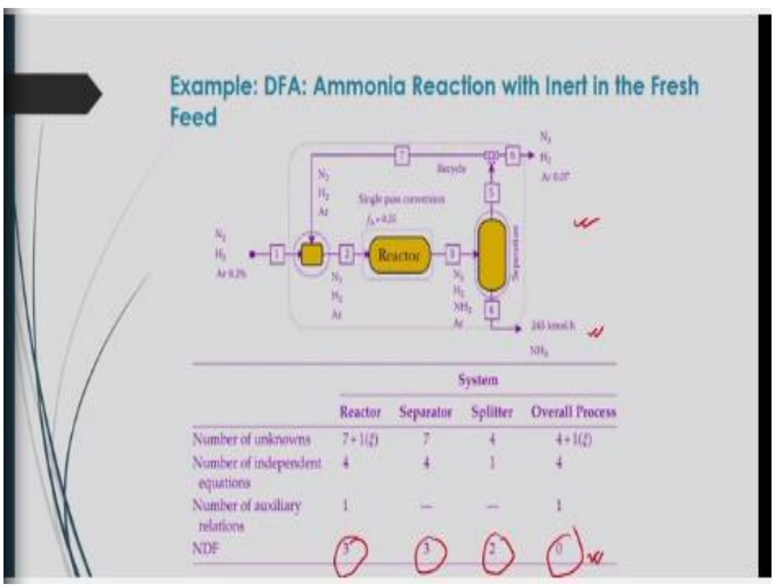

	System			
	Reactor	Separator	Splitter	Overall Process
Number of unknowns	7+1(ξ)	7	4	4+1(ξ)
Number of independent equations	4	4	1	4
Number of auxiliary relations	1	–	–	1
NDF	3	3	2	0

And here all the you know knowns and unknown you know variables specified in this flowchart in it is you know respective you know flow streams and respective you know units. And they are respective you know degrees of freedoms are analyzed for individual units like this. Here also you are getting that overall process this degrees of freedom is 0, so we can say that these systems can be you know well defined well specified. So you can solve this equation to get the unique solution.

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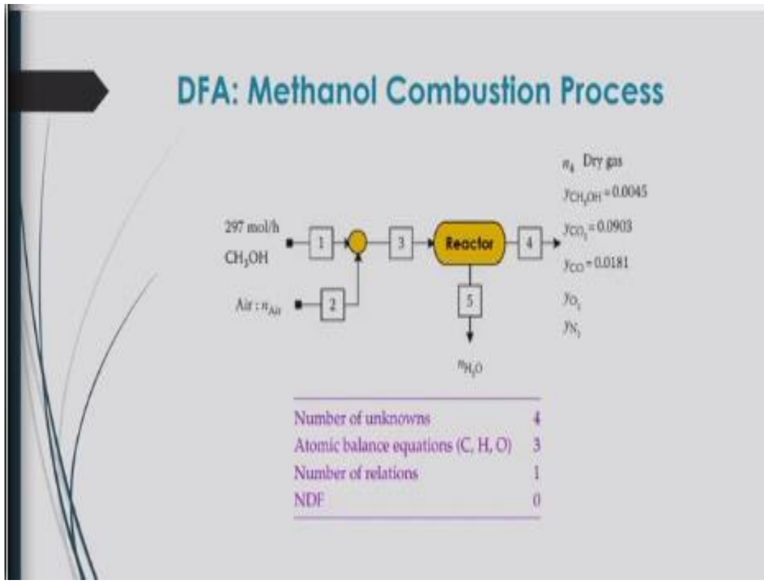

Another example, methanol combustion process how to analyze the degrees of freedom. Here also you can get this degrees of freedom as 0 with this known and unknown variables in the flowchart.

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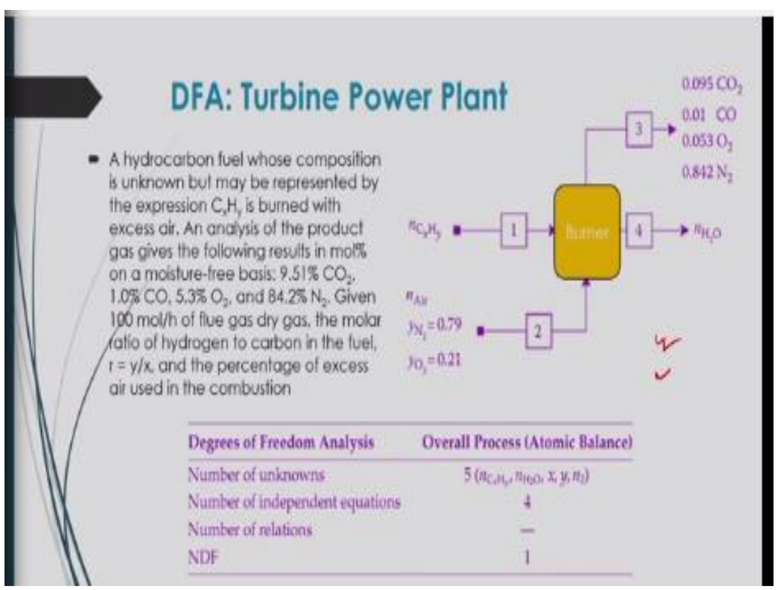

Similarly turbine power plant how to do the degrees of freedom analysis it is given. Please go through this again the basic concept is to that use that you know definition of degrees of freedom and to find out that number of unknowns, number of independent equations and relations and accordingly what should be the number of degrees of freedom. So here it is given this examples please go through these examples and try to understand how to calculate this degrees of freedom there.

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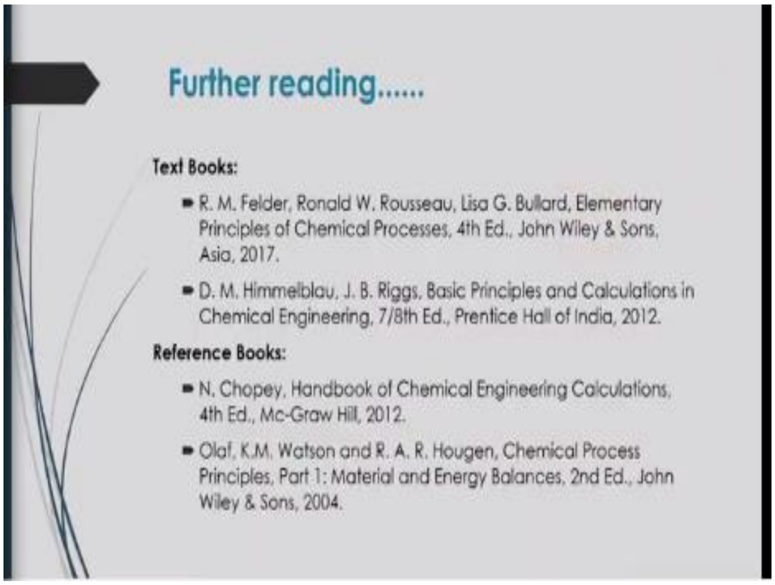

So, I would suggest you to go further reading for this analysis of degrees of freedom this textbooks is given here even you can follow the reference books also for this analysis.

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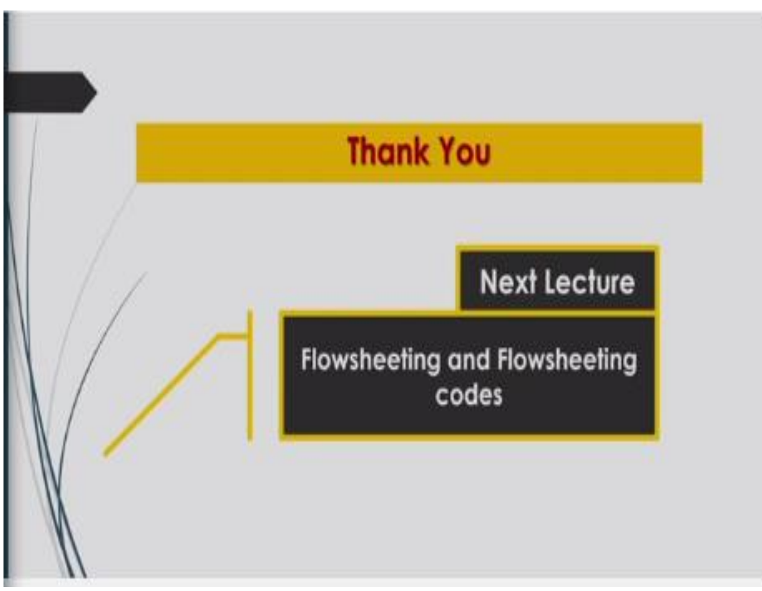

So we will discuss more about this computational flowsheet based on you know our material balance equations analysis. In the next lecture we will describe about flowsheeting and flowsheeting codes there under this same module. So thank you for your attention here.