Material and Energy Balance Computations

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Lecture –07

Fundamentals of Material Balance (Contd.,)

Hello everyone, and welcome back to another class of Material and Energy Balance Computation. We are in module 2 that is the material balance calculations and its fundamental and application to the single unit. We will continue our discussion from the last class where we were discussing the general balance application to the continuous process that we have seen in the last class, and now we will see its application on the batch processes.

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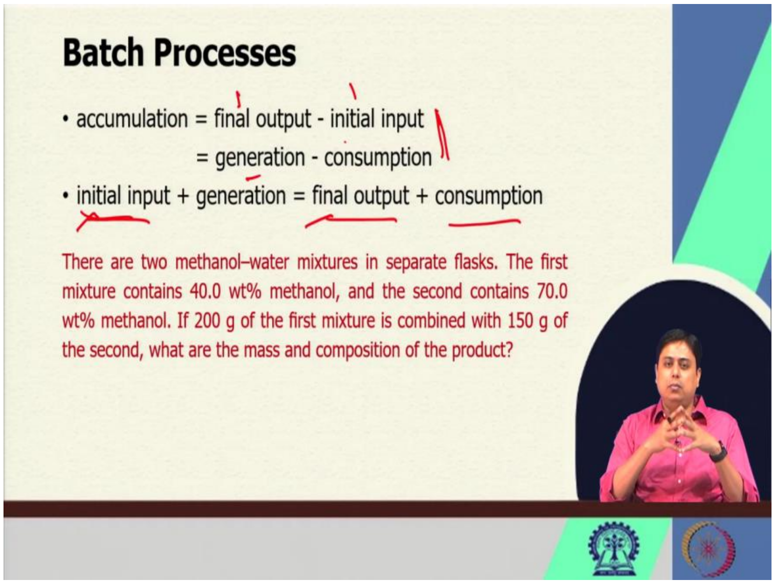

Batch Processes

- accumulation = final output - initial input
  = generation - consumption
- initial input + generation = final output + consumption

There are two methanol–water mixtures in separate flasks. The first mixture contains 40.0 wt% methanol, and the second contains 70.0 wt% methanol. If 200 g of the first mixture is combined with 150 g of the second, what are the mass and composition of the product?

Now in a batch process, as I mentioned earlier, it is the report that we understand between two instants in time that is in a time interval. So say, for example, you have nitrogen and hydrogen in an ideal reactive condition that can produce ammonia. Now, these two streams, nitrogen and hydrogen are fed into the reactor where the desired temperature, pressure and everything is set in order to convert those to ammonia.

Now we charge or we keep those nitrogen and hydrogen in that reactor. And then leave it for some time for the reaction to complete, and after a certain time we take out the product ammonia. Now, in this case, you can understand that in between this period that when we place or keep those two streams or two material two species that is nitrogen and hydrogen in the chamber and then we take out ammonia after some time in between that we did not take out any ammonia.

So that means in this case, what is happening is that ammonia is being generated, and it is also being accumulated. So that means we have a generation of ammonia = the accumulation of ammonia. So that means what we can understand about the accumulation. It is basically the final output – the initial input. Now for the case of ammonia, there was no initial input. Now here remember the terminology that we have mentioning here it is the final and initial.

This is to demarcate the time interval or 2 instants of time. Initial means when we charge the reactor with the species. Now if there is pure nitrogen and pure hydrogen, there is no Ammonia initially, that concentration is zero. So that means accumulation the way we understand is the final output – initial input. Now at the same time, so if we now look at our generic balance expression. From there we can see that accumulation is also the generation – consumption.

So it is the amount or the difference between it is generated and being consumed. So that means based on these two since these both results result in accumulation, what we can write is that the initial input + generation = final output + consumption. So this is, in fact, the similar kind that we have seen in the case of continuous operations and there instead of the initial input, it was simply written as input + generation is equals to output + consumption for the continuous process.

But now here again since the time interval is involved. It is not a continuous process. So it is now the initial input it means the amount of the balanced material of the balanced parameter that we are writing here. So accordingly we choose our unit. The generation is the amount of things that is being generated, not per unit time. So now the point is that it is similar to the case that we have seen in the case of the steady-state continuous process except these 2 terms that is the initial and the final input and output.

So say we have two mixtures of methanol and water in 2 separate flasks. Now one mixture contains 40 wt % methanol and the second one contains 70 wt % methanol, and now if we mix 200 gram of the first mixture with 150 gram of the second mixture, what would be the mass and composition of the product? A simple problem, but it is necessary to understand this concept of its application in the context of a batch process.

Again our first task could be to schematically represent this problem so that we can quickly visualize what is happening?

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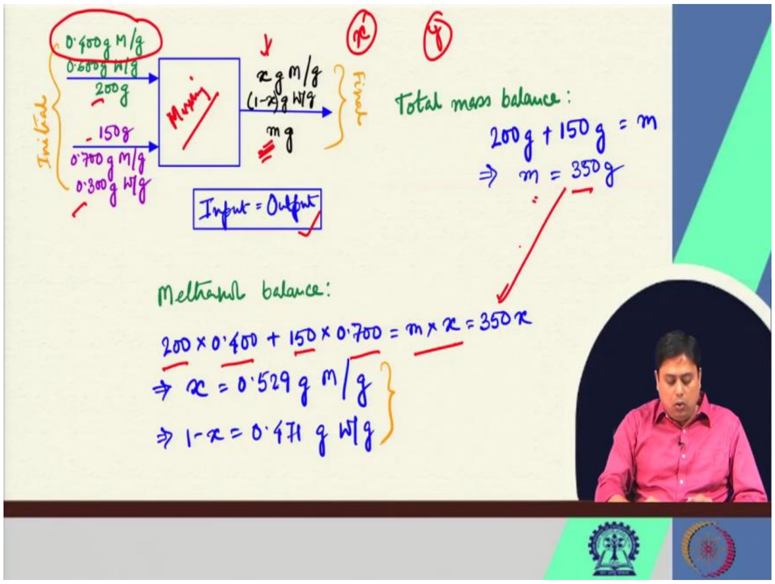

So if we try to interpret that in a schematic, it would look like this. That we have mixing process or operation that is happening here. Where there are two streams or two substances that are being mixed in batch. One is of 200 gram and the other one is of 150 gram. Now this 200 gram contains as a problem statement say 40 wt % methanol. So that means rest is the water so m stands for the methanol and w stands for the water.

So, this is how we can write the composition on this schematic. Now here the point is that if you notice the problem statement says 40.0 wt % methanol, 70.0 wt % methanol in the second stream that means there is an emphasis on the significant digit and that is why to the 3 decimal point here it is written as 0.400 gram of methanol per gram of the mixture of the first stream and similarly for the second stream we have 150 gram in which we have 0.700 gram of methanol per gram of this stream which is the 70% by weight and that means 30% by weight we have water in the second stream or the second mixture.

These two are being mixed. We do not know what is the product? So what is the weight of the product now this is a very simple problem. So we know that eventually to be the 350 gram of mixture that is coming out, but we do not know its composition. So the composition we assume that there will be x gram of methanol per gram of the mixture of the product mixture. So that means 1 – x gram would be our water concentration.

Now here, if you look at the problem statement, it is based on the weight the percentage is given. And so that is why it is written here x because if you remember a couple of classes earlier, we mentioned that the weight fraction will be mentioning by x and the mole fraction we will designate by y. So here it is the weight fraction that means gram of methanol per gram of the mixture, the gram of water per gram of the mixture. So, the total mixture is, but we have the m gram. Now there is no reaction happening ok and just before this slide we have seen, this is the balance equation in case of a typical batch process that is the initial input + generation is equals to final output + consumption or there is no generation and no consumption because its non-reactive species.

So we ended up with simple input = output. Now say we apply this, now the easiest part is to have the total mass balance because now we understand that this has to be conserved at the first place. So that means the total mass of the product would be 350 gram. And then say we apply this to methanol, one of the species. We can apply to water as well. But say in this case we have applied this to methanol balance.

So methanol balance input = output around this mixing or into the mixing chamber what we have 200 gram of one stream where we have 40 wt % of methanol + 150 gram of the second stream where we have 70 wt % of methanol. Now, this total methanol has to be conserved because it is input = output. So, in the output stream, we have the amount of the output stream and its concentration that is the weight percentage of methanol in it, which is x is the unknown.

We just calculated the value of m, So we can easily calculate the value of x that will have a unit which is 0.529 gram of methanol per gram of the output stream, the output mixture. Which means the 1 – x would be the water weight percentage. Now, here again, it has been tried to preserve or to follow the significant digits calculation, and it is reported in that fashion. So which means we have 52.9 wt % methanol in the output stream and 47.1 wt % of water in that stream of the in that output.

Now it is preferable that we do not mention for the stream in the case of the batch because stream kind of sounds like it is a flowing or a continuous operation. So instead of that we from now on will mention as say the output only on the input feed or the output in the case of a batch process. So this is how a simple material balance with this example of the simple material balance as we have seen that how this is generic energy balance equations are applied and what would be the nature of such calculations in future?

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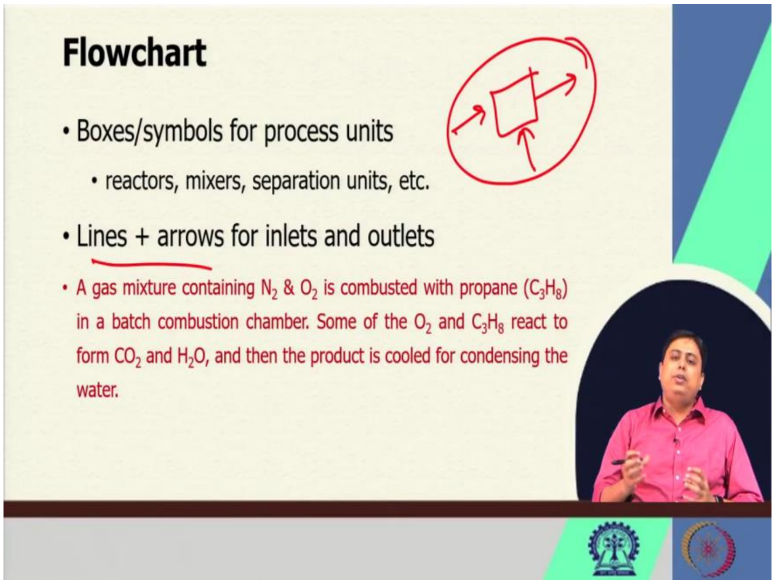

Flowchart

- Boxes/symbols for process units
  - reactors, mixers, separation units, etc.
- Lines + arrows for inlets and outlets
- A gas mixture containing N_2 & O_2 is combusted with propane (C_3H_8) in a batch combustion chamber. Some of the O_2 and C_3H_8 react to form CO_2 and H_2O, and then the product is cooled for condensing the water.

Now as I mentioned the first task in solving this material or the energy balances is to draw the schematic and technically we call that as flowchart in such process calculation. Flowchart means that we represent the process units such as reactors mixture or separation units by boxes or certain type of symbol. For those detailed outlining of symbols will not go into their; we will just represent those as simple boxes.

But reactor mixture and separation units have their own symbols when it comes to commercial application. So that they can be easily identified with that is a reactor with that is a mixture that is a separator. But since we are just understanding the basics, we will just represent any separating unit or any processing unit to say by a rectangular or a square box. And the inlets and outlets we will represent those with the combination of lines and arrows.

So something comes in, something goes out if there are two streams coming in, we have such kind of conventional schematic notations these are called the flowchart. Now the point is that say why it is needed? Since this couple of initial classes or focused on the single unit balance, we are mainly focused on only one stage of operation, but as I mentioned earlier, this process operations is hardly a single-stage process.

It is a cascade of operations that follows one after another. Now there are different process variables different process conditions that are maintained for each and every unit. And those would be given to you in kind in the manner, for example, one of the small example that is shown here. So say a gas mixture containing nitrogen and oxygen is combusted with propane in a batch combustion chamber.

Some of the oxygen and propane react to form carbon dioxide and water, and then the product is cooled where the water is condensed. Further, that condensed water may go to another process operation where something or the other will happen there. So the problem statement will be going in a lengthy fashion. So it would be difficult for us to remember what was happening in the first stage of operation.

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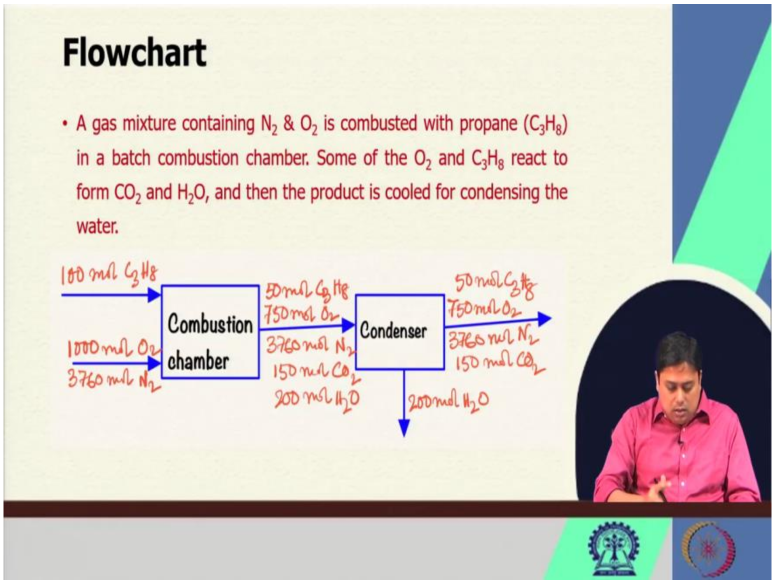

Flowchart

- A gas mixture containing N_2 & O_2 is combusted with propane (C_3H_8) in a batch combustion chamber. Some of the O_2 and C_3H_8 react to form CO_2 and H_2O, and then the product is cooled for condensing the water.

So the utility of this flow chart is that we quickly present the whole problem systematically so that we further need not look back to the problem statement to get those data or to understand the process condition or the process parameters. So, for example, this is the flowchart representation of the problem statement that I just read. So we had a combustion chamber, where two streams were coming. Now, these streams it is the mole fraction or the composition what was not mentioned in the problem statement, but those will also be mentioned.

So those also we write immediately on the flowchart. But how much mole or how much molar flow rate is there but since this is a batch operation, there will not be a flow rate amount would be there only. So two substances or say one mixture and the other pure substance is charged into a combustion chamber. Now it is said that sum of O_2 and C_3H_8 would react to form CO_2 and H_2O, that means some of the reactants would also be there that unreacted reactants.

We must write those as well so that we do not miss those parameters later. And then the whole mixture is going to a condenser where water is condensed from the streams that means here we will have the rest of the components in the output stream or say in the output itself because it is the batch operations will try to avoid the stream. Now, as I mentioned, this problem statement could be further lengthier if something is mentioned that now these components are further taken to another reactor for subsequent reaction to happen. So this is how a flow chart is mandatory, and it is very essential.

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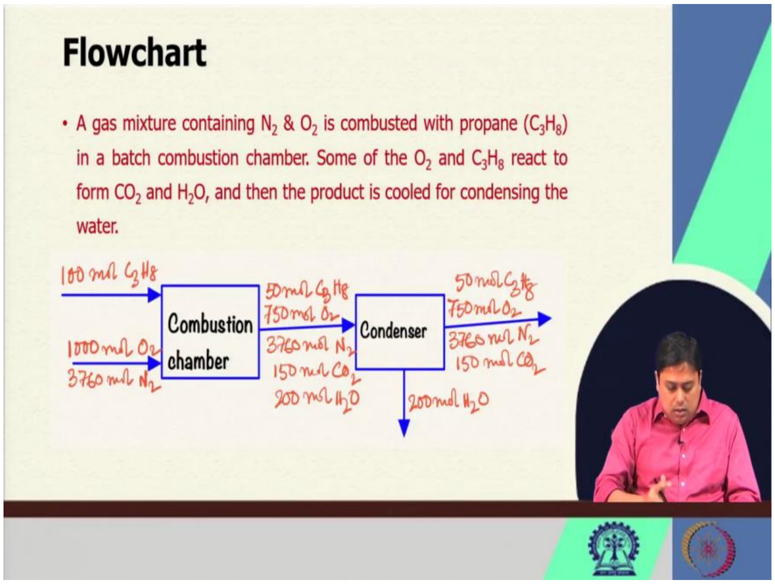

Flowchart

- A gas mixture containing N_2 & O_2 is combusted with propane (C_3H_8) in a batch combustion chamber. Some of the O_2 and C_3H_8 react to form CO_2 and H_2O, and then the product is cooled for condensing the water.

There are few conventions that we should follow. And the flowchart sho9uld be as detailed as possible, which means we will try to write each and every process condition and the process variable that are available in the problem statement. So for example this green arrow represents inlet or outlet stream or input or output in the case of batch operations. Now here specifically, it is per hour flow rate is mentioned.

It is mentioned as flow rate that means it is for a continuous operation. This is how we identify. So, in this case, we have a flow rate that is mentioned the total flow rate of this stream in which the molar composition is mentioned that means it is air here in which we have 21-mole percent oxygen and 79-mole percent nitrogen. So, it is flowing at a temperature and also a known pressure. This is how the detailed labelling should have been so that if some process unit is here, it is entering into the process unit and leaving with the different temperature and pressure.

So that we can quickly understand that there is a difference in temperature and pressure we have to account for. If you do not mention these process conditions in detail, we may miss these points while doing some critical calculations. Now the point of detailing can also be realised here, that how do you represent the data that is given in the problem statement. So, for example, it is mentioned we have 60-mole percent nitrogen and 40-mole percent oxygen or say 60-mole percent nitrogen and the rest oxygen is flowing in a stream.

So if nothing further is mentioned, we can assume that we have 100 mol/min of flow rate that is happening or if it is also given, then the same thing can be represented in this fashion as well. That means 60 mole of nitrogen per minute is the flow rate of nitrogen and 40 mole of Oxygen per minute is the flow rate of oxygen because we have 100 moles of minute flow rate of the mixture and where we have 60-mole percent nitrogen and 40-mole percent oxygen.

So someone can write the flowchart in this fashion as well as the others also can write or they can also write in this fashion as well. Both represents the similar information's or the identical information's but in a different way.

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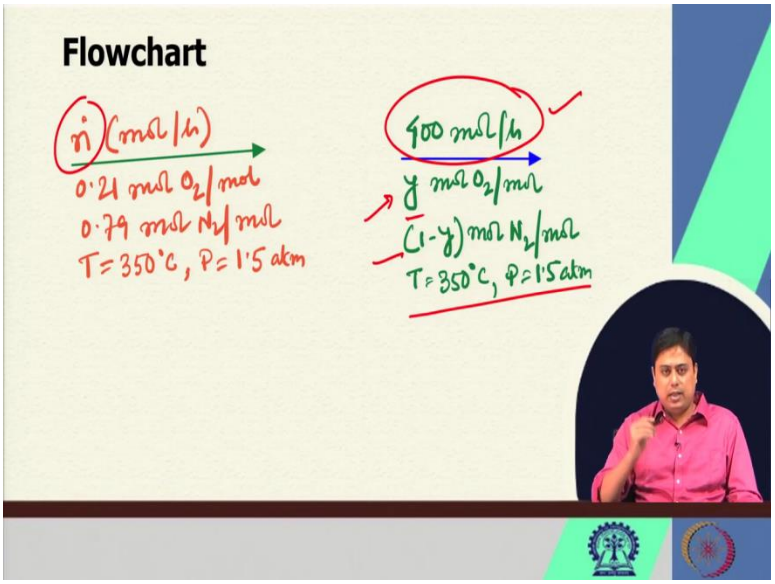

Flowchart

$\dot{n}$ (mol/h)

0.21 mol O_2/mol

0.79 mol N_2/mol

T = 350°C, P = 1.5 atm

400 mol/h

y mol O_2/mol

(1 - y) mol N_2/mol

T = 350°C, P = 1.5 atm

When we have unknowns or we do not know what is the certain variable or parameter we typically represent that with the unknown parameters. For example, if that is a flow rate we give the nomenclature that is of dot on top of it is a molar flow rate n is the number of moles ṅ is the molar flow rate that is the mol/h. If, say, the total molar flow rate is known but the composition is unknown, the convention is that we assume y as the mole fraction because you remember the difference between defining x and y.

x is the weight percentage, y is the mole percentage, and this is the convention we will follow.

So since it is the molar flow rate we write this as y moles or we assume the composition as y moles of oxygen per mole of the mixture or the mole of the output stream or inlet stream whatever that be and the rest is nitrogen if it is simply air and no other composition is mentioned. And again we should not forget to write the process conditions as well because these are also process variables, which can change from input to output.

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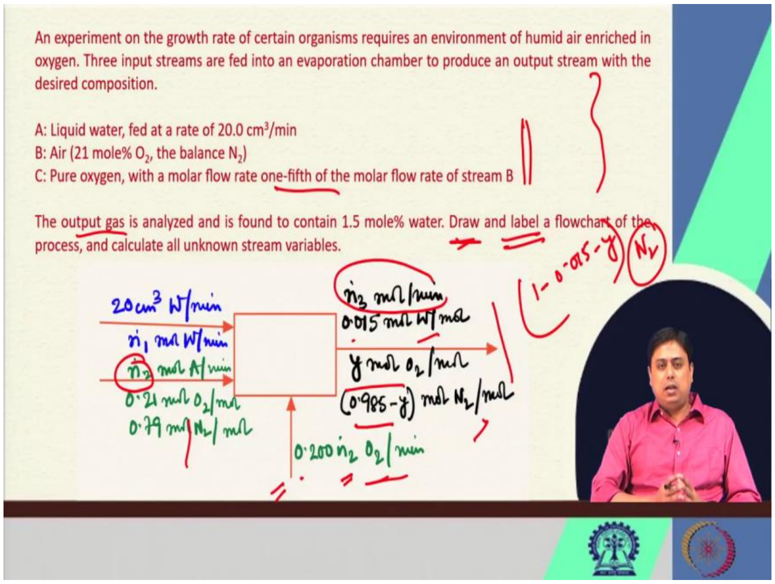

An experiment on the growth rate of certain organisms requires an environment of humid air enriched in oxygen. Three input streams are fed into an evaporation chamber to produce an output stream with the desired composition.

A: Liquid water, fed at a rate of 20.0 cm^3/min
B: Air (21 mole% O_2, the balance N_2)
C: Pure oxygen, with a molar flow rate one-fifth of the molar flow rate of stream B

The output gas is analyzed and is found to contain 1.5 mole% water. Draw and label a flowchart of the process, and calculate all unknown stream variables.

So say we have a scenario that an experiment on the growth rate of certain organisms requires an environment of humid air enriched in oxygen. Now so this kind of certain organisms are say the yeast and several other things that can happen, but what is important here is that we need, say 3 input streams into an evaporation chamber to produce an output stream with the desired composition and those input streams are these three streams.

That is the liquid water that is fed at a rate of 20 cm^3/min, the air we have 21-mol % oxygen and balance nitrogen. And the third stream is pure oxygen which is having a molar flow rate that is one-fifth of the molar flow rate of stream B. Output gas is analysed and it is found that we have 1.5-mole percent water in that output stream. So our job is to find out all unknown stream variables and before that, we have to draw and label a flowchart of the process.

So this is how a problem statement would look like, and it is the onset of making it complex that now the stream compositions are connected or the unknowns are connected with the other stream. And the utility of drawing flowchart is prominent further. So here again, this is focused on only a single unit. So we have stream A where we have 20 cm^3 w/min , w stands for water. That means we have $\dot{n}_1$ mole of water per minute.

The second stream contains air the molar flow rate is not known so we designate that has $\dot{n}_2$ and another unknown molar of A stands for the air per minute which has a composition of 21-mole percent oxygen that is 0.21 mole of O_2 per mole of air and the rest is nitrogen. The third stream is pure oxygen that has a 1/5 times molar flow rate that to of stream B. Now in the case of stream B, we just assume just one variable one can always assume here another variable, but then he must immediately write the relation between this $\dot{n}_2$ and this new variable that he or she is defining.

Or the other way is that we directly write as per this relation that it is 1/5 that means 0.200 in 2 times or $\dot{n}_2$ times O_2 is the flow rate of this stream. We have the output this output again the molar flow rate is unknown. So we define another variable there. There is one known thing there that we have 1.5-mole percent water that means 0.15 mole of water per mole of this output stream. Now should I leave it there of course not because although it is not clearly mentioned that output gas, what are the components it is comprised of it is quite logical that now here we have water and air.

And the output stream we just mentioned only water component so which means we will have this individual species that is oxygen and nitrogen also in the output stream because no reaction is happening. So that means we have to assume the mole fraction of oxygen and the total mole fraction sum of these three components should be one so that means one can also simply write that 1 – 0.015 – y is my N_2 concentrations or the number of mole of nitrogen per mole of this outputs stream.

This is how we draw and label of flowchart. Just drawing the flowchart is not sufficient, we have to label it as soon as possible and with every detail that is given. So with this I will stop here and will take up this problem further in the next class where we will see how to solve such problem as well. But the take-home message from this lecture is that flow chart drawing is essential, and it should be done even if the problem statement is explicitly not mentioning it.

And as soon as we draw the flowchart, we must label it to the full detail that is given in the problem statement, with this; I stop here and thank you for your attention.