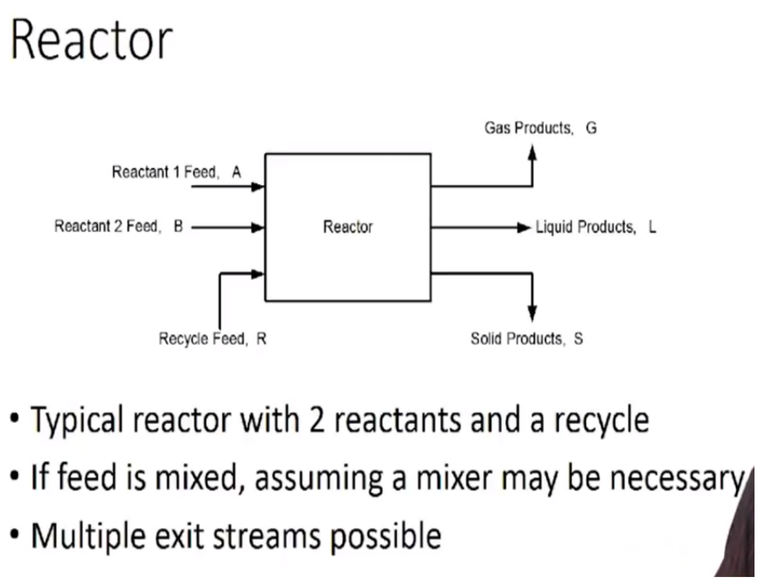
Material and Energy Balances

Prof.Vingesh Muthuvijayan
Department of Biotechnology
Indian Institute of Technology – Madras

Module No # 03
Lecture No # 11
Material Balance Calculations For Single Units With A Single Reaction

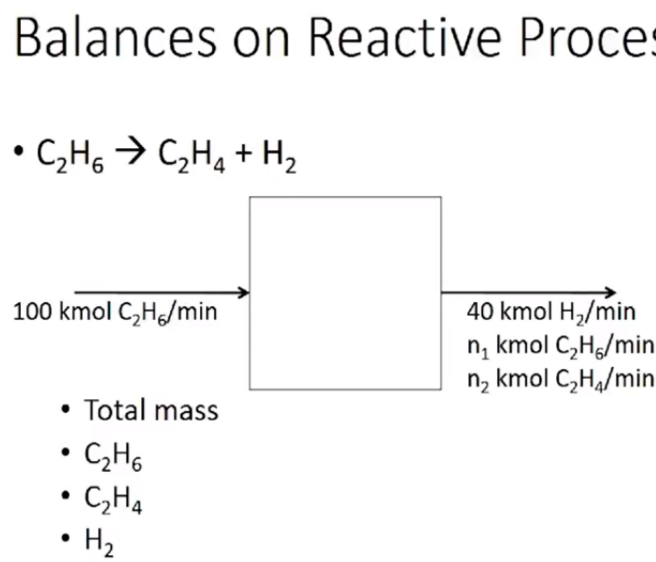
Welcome to today's lecture on material balance calculation for single unit system with reactions so to start with we have now understood the fundamentals associated with reactive processes and terminologies which will be used when we discuss processes having reaction and reactors. So we will start off with simpler possible systems which have reactions which are single unit systems containing only single reaction what we will do is we first try to understand what a reactor is and we will look at different ways to write balance equation for this type of the system.

(Refer Slide Time: 00:55)



What is a reactors? The diagram you see here is typical represent of a reactor which as two feeds and cycle you can have products it could be gas products or liquid products or solid products these products could be coming out as different streams and they can actually be separated further.

(Refer Slide Time: 01:16)

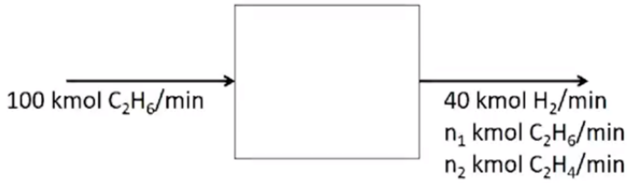


Consider these reaction which is shown here have ethane forming ethylene and hydrogen. So the reaction system is written as 100 kilo moles of ethane entering per minute reacting to form 40 kilo moles of hydrogen per minute. We do not know the number of moles of ethane and ethylene which are leaving the system. Now that we have the system what kind of balances we write when we looked at water conserved we identified that the mass of the total substance and the mass of the individual components could be consent.

So we write the total balance which is the total mass balance and also we write individual component balances which would be the ethane ethylene and hydrogen balances. Let us see how these equations would look and how we can solve for N1 and N2.

(Refer Slide Time: 02:06)

Balances on Reactive Processes



Basis - 100 kmol C_2H_6/min

Total mass: $100 \times 30 = 40 \times 2 + n_1 \times 30 + n_2 \times 28$

C_2H_6: $100 = n_1 + \text{consumption}$ $\quad I - O + G - C = A \Rightarrow I = O + C$

C_2H_4: $Gen_E = n_2$ $\quad I - O + G - C = A \Rightarrow O = G$

H_2: $Gen_H = 40$

Find n_1 and n_2 using stoichiometry and these balances

So we now have the reactions system and we can write the total balance before that we need to identify the basis for the system. For the given condition we have the 100 kilo moles of methane entering which means the basis would be 100 kilo moles of ethane per minute. Now the total mass balance written in terms of masses not in terms of moles as we already looked at mass is conserved number of moles is not conserved during a reaction.

So the total mass would be written as 100 kilo moles of ethane times the molecular weight of ethane which is 30 is the input mass and you have the output mass as 40 times 2 representing the mass of hydrogen leaving the system and N1 times 30 representing the mass of ethane leaving the system and N2 times 28 which is the mass of ethylene leaving the system. Now we can also write ethane and ethylene balances.

Ethane balance is 100 moles entering and this is equal to N1 moles which is leaving + consumption so this equation basically comes down from input – output + generation – consumption = accumulation assuming steady state accumulation goes to 0. Now we have input term for ethane and we know that 100 kilo moles of ethane is entering there is also an output term because we know that N1 kilo moles of ethane is leaving the system is there a generation term no because this is a reactant.

So the generation term goes to 0 however we still have a consumption term so this means the equation comes down to input = output + consumption which is what we have written here which is N1 + consumption for ethylene the equation comes down to input – output + generation – consumption = accumulation.

Accumulation going to 0 because of steady state and there is no consumption because this is a product is only being produced you do not have any input this implies you have output = generation this is what we have written as generation = N2 which is the output. Similarly for hydrogen we can write the balance equation as generation = output which is 40 kilo moles per minute.

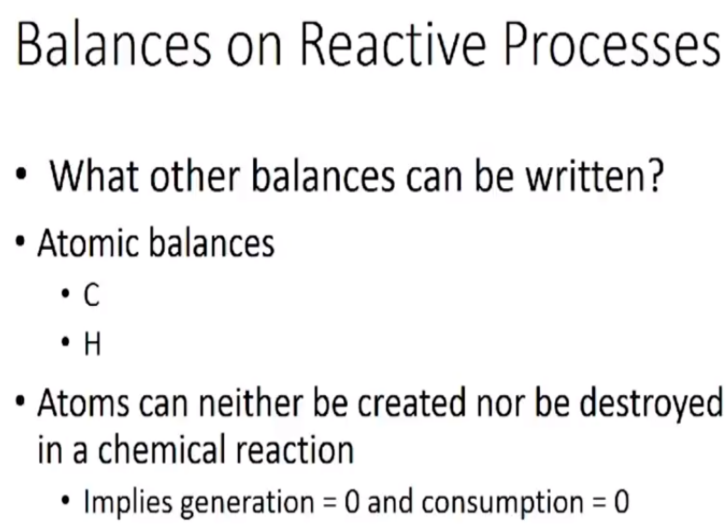
One thing you would have observed the when we write the total to mass balance I have converted all the moles to mass this however when I wrote the individual component balances I did not bother to convert the moles to masses why the reason is simple you actually be multiplying all these molecular all these moles by molecular weight to convert them into masses.

So each of these terms would be multiplied by the molecular weight of the particular component which can get cancelled off this would lead to finally the same equation so that is why we did have to convert to mass for individual components. Now that we have 3 equations we can easily solve for the two unknowns and we will be able to get the final value.

So we can actually use to stoichiometric to know that for every mole of hydrogen produce you would have one mole of ethylene also to be produced. So using that you can identify the generation of ethylene and that will give you the output of ethylene which is N2 and similarly you can know the consumption of ethane using the stoichiometric.

So one mole of ethane results in the formation of one mole to hydrogen so which means 40 moles of ethane as to be consumed to produce 40 moles of hydrogen. So substituting that you would be able to get the value of N1 also so using stoichiometric and these balances we can actually calculate N1 and N2.

(Refer Slide Time: 06:18)

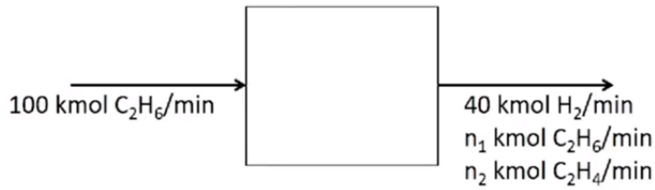


Other than these molecular species balances what are the balances we can write if you remember the fundamental which we cover for reactive processes we sort that other than mass the number of atoms of individual elements are also concerned which means we can write atomic balances for this particular system we have carbon and hydrogen atom which are present and the balance of hydrogen atom can be written.

Let us see how about going to that so first think we need to understand is atoms can either be created or be destroyed in a chemical reaction. That is why the number of atoms carbon in the reactants is same as the number of atoms on your product. So this implies generation in consumption terms will be always be 0 for atomic species balances as we always assume steady state accumulation will be 0 so the equation simplifies to input = output also be 0.

(Refer Slide Time: 07:18)

Balances on Reactive Processes



C: $100 \times 2 = 2 \times n_1 + 2 \times n_2$

$100 = n_1 + n_2$

H: $100 \times 6 = 40 \times 2 + 6 \times n_1 + 4 \times n_2$

$520 = 6n_1 + 4n_2$

Solve for n_1 and n_2

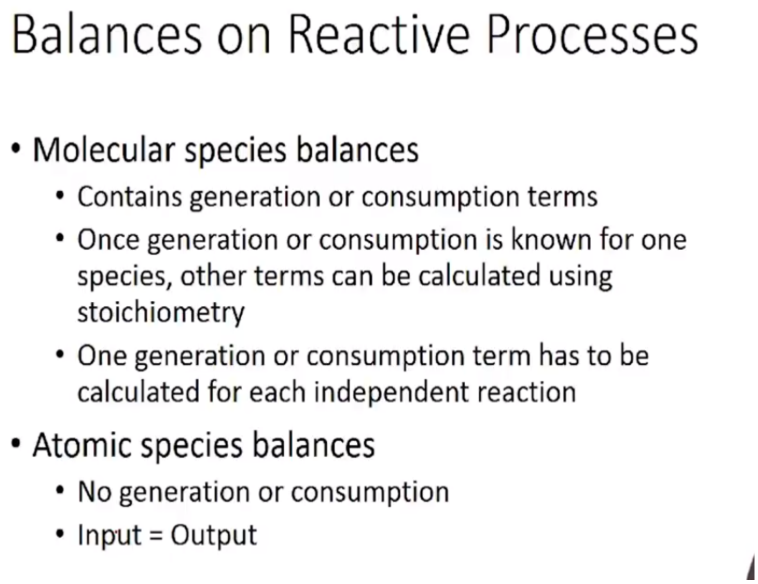
Now let us look at the same example problem and see whether we can write atomic species balances and arrive at the same answer. Carbon balance would look like this you have 100 kilo moles of carbon entering we will be multiplying with 2 because with each mole of ethane entering two atom of carbon is also entering so each molecule of ethane you have two atoms of carbon.

So when we convert 100 kilo moles of ethane we would actually have 100 times 2 kilo moles of carbon entering the system so that is your input and your output would be carbon leaving through ethane and ethylene both ethane and ethylene have two atoms of carbon each so we have two times N and two times N2. Similarly we can write a balance equation for hydrogen which would look like this.

100 times 6 equals 40 times 2 + 6 times N1 + 4 times N2 so what you can see here is you have 6 atoms of hydrogen entering through one molecule of methane and two atoms of hydrogen entering through 1 molecule of hydrogen 6 atom of hydrogen entering through one molecule of leaving through one molecule of ethane and 4 atoms of hydrogen is leaving through 1 atom of ethylene.

So substituting all these values you end up with 520 = 6N2 + 4N2 we now have two equations and two unknowns these can be used to solve for N1 and N2. So these are two approaches through which we can solve material balances for reactive processes.

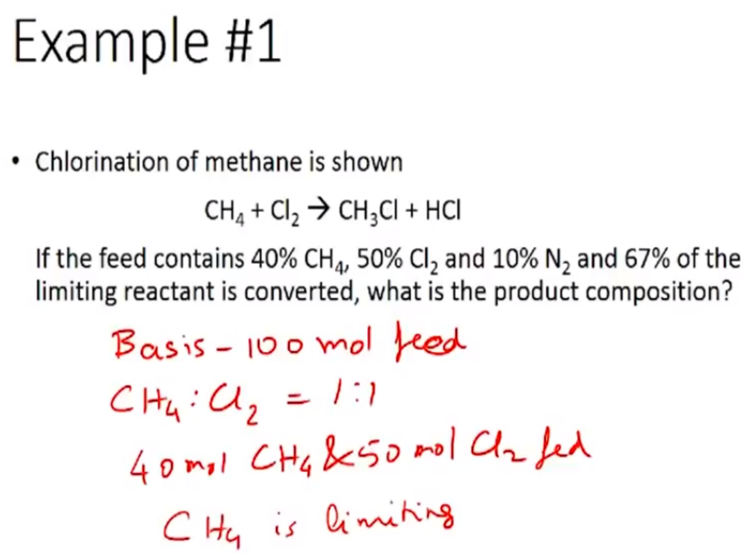
(Refer Slide Time: 09:09)



So the first technique which we used is called as the molecular species balance this will contain and generation or an consumption term depending on whether you are writing an balance for a reactant or a product. Once a generation or consumption term is known for one of the species other terms can be calculated other generation or consumption terms can be calculated using stoichiometric.

Once generation or consumption term as to be calculated for each independent reaction only then you will be able to calculate the consumption and generation for each of the task. We also can write atomic species balance which is second type of balances which we wrote. Here we do not have generation or consumption term so the equation simplifies to input = output.

(Refer Slide Time: 09:58)



Now that we have the fundamentals let us look at the example problem chlorination of methane is given by the reaction methane + chlorine giving CH3CL + HCL if the feed contains 40 % methane 50% chlorine and 10 % nitrogen and 67% of the limiting reactant is converted what is the product composition ? So now this problem uses fundamental terminologies which we learnt in the previous lecture let us see how we can solve this problem.

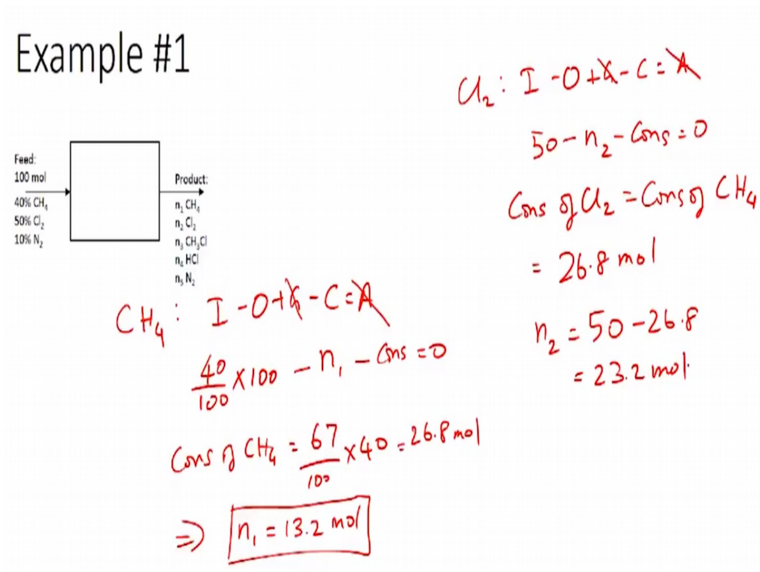
The first thing you see in the problem is no mass or mole flow rates is given in the system which means we would have to assume the basis as the composition are given in terms of percentages we can use to 100 moles as the basis why do we choose 100 moles? If you remember I had mentioned in one of the earlier lectures that in general mass percentages are used for solids and liquids and mole percentages are used for gases.

So here the composition which is given is for a gas which would mean the percentages which is given are for mole percentages and thereby we use 100 moles per basis instead of using a mass based basis. So let us start solving the this problem so basis is identified as 100 moles of feed and we know that the stoichiometric ratio of methane to chlorine is 1 is to 1 so based on the basis we have calculate that 40 moles of methane and 50 moles of chlorine are entering into the system.

So this implies that methane is you limiting reactant as it is provided at a lower stoichiometric amount. So we will have to write balances equations so let us try to write the balance equation for the total mass or components. Now that we have identified methane is the limiting reactant we can write balance equations if you were to write the total balance equations we would not be able to get the much equation as we would have lot of unknowns in that equation.

So instead we can start with the component balances and try to solve this equations independently.

(Refer Slide Time: 12:34)



So this particular diagram represents the process which we are looking at so let us write the mass balances for each of the component. So for methane the system would the balance equation would look like input – output + generation – consumption = accumulation assuming steady state accumulation goes to 0 methane is actually taking part in reaction it will just get consumed it will not get generated so generation goes to 0 you have both input and output terms.

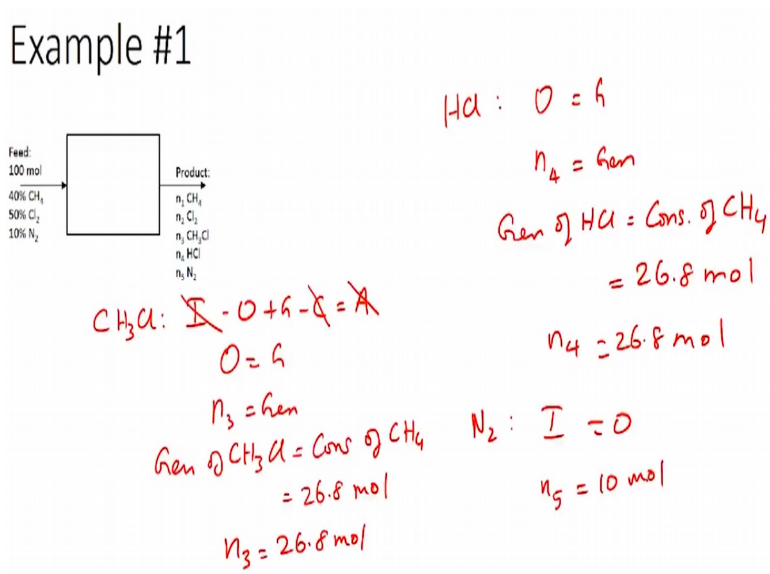
So this would mean your input term which is 40% of 100 giving you 40 moles which is coming in – output term for methane we have assume to be N1 – consumption of methane = 0 can we calculate the consumption of methane. We know that methane is the limiting reaction and the problem statement says that 67% of limiting reactant actually gets converted which means consumption of methane would be 67% of 40 moles which is fed giving you a value of 26.8 moles.

So this implies we can substitute this values for consumption and calculate the value for methane leaving the system as 13.2 moles. So this gives you the number of moles of methane leaving the system. Now we can write a balance equation for chlorine so again you would have input – output + generation + consumption = accumulation. Assuming steady state goes to 0 chlorine is not produced in the reactions which means generation would goes to 0.

So you are only left with input output and consumption we know that the input term is 50 moles of chlorine entering for the basis of moles and the output is given as N2 moles and the consumption is needs to be calculated so what is the consumption of chlorine that needs to be calculated we know that for every mole of methane consumed one moles of chlorine would have also been consumed that is based on the stoichiometric ratio of methane and chlorine in the reaction.

So this mean the consumption of chlorine would be equal to consumption of methane thereby giving you a value of 26.8 moles of chlorine is being consumed. So substituting it back into this equation you will get M2 as 50 – 26.8 giving you 23.2 moles.

(Refer Slide Time: 15:36)



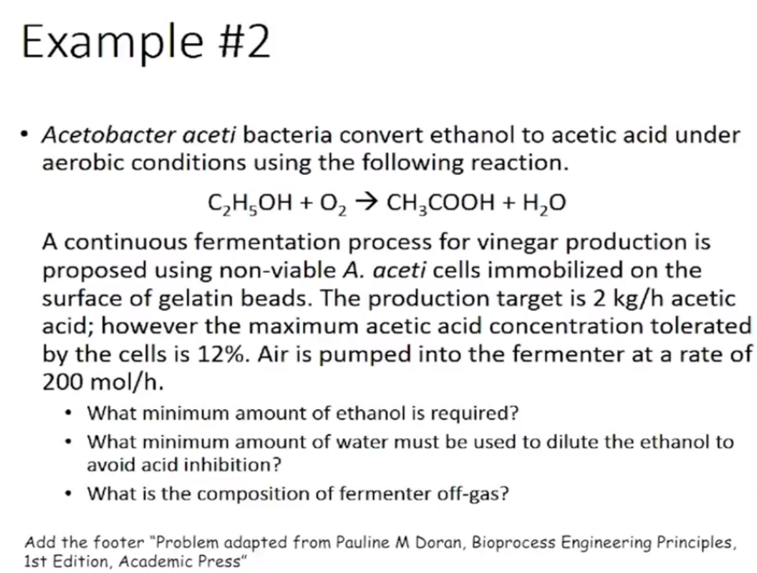
Now that we have calculated the outlet streams for the reactants you will start with the other products which are formed this reaction and also the inert which is entering and leaving the reactants. So now you will write a balance equation for CH3 CL so again we will start with input – output + generation – consumption = accumulation. Accumulation goes to 0 so this is a product so there is no consumption is only generation there is now input of CH3CL.

So you have left with output = generation so your output which is N3 = generation so now we need to know the generation of CH3CL is. So based on the stoichiometric we know that for every mole of methane consumed one mole of CH3CL is formed which means the generation of CH3CL would be numerically equal to consumption of methane = stoichiometric there by generation of CH3Cl is given as 26.8 moles.

So this means we end up with N3 = 26.8 moles now we can write the balance equation for HCL for HCL you would again have the equations simplified to output = generation just like how we did for CH3CL so you will N4 = generation again using stoichiometric generation of HCL = consumption of CH4 methane which is 26.8 moles. So this implied N4 is 26.8 moles. So the final term which we need to calculate is the number of moles of nitrogen entering and the leaving the reactants.

Nitrogen does not take part in the reaction so there should not be any generation of consumption terms and as we do not have accumulation under steady state the nitrogen balance is very simple which is input = output thereby giving the output N5 as same as output which is 10 moles. So with this we have calculated the number of moles of each of the component balance which are leaving the system.

(Refer Slide Time: 18:08)

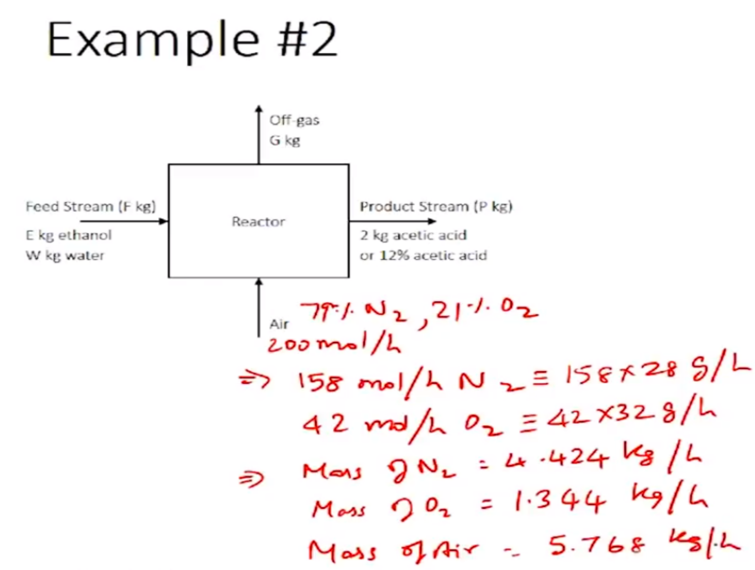


Let us now move on to another example problem Acetobacter aceti which is a bacteria can convert ethanol to acetic acid under aerobic conditions so the reaction is given as ethanol +

oxygen forming acetic acid + water. A continuous fermentation process for vinegar production is proposed is using non-viable acetobacter aceti cells immobilized on the surface of gelatin beads.

The production target is 2 kilogram per hour of acetic acid however the maximum concentration of acetic acid that is tolerated by the services is 12% air is pumped into the fermenter at a rate of 200 moles per hour you are expect to calculate the minimum amount of ethanol is required minimum amount of water that must be used to dilute to the ethanol to avoid acid inhibition and the composition of fermenter half gas.

(Refer Slide Time: 19:06)



Let us look at solving this problem so we have a reactor with an input that contains ethanol and water which is called the feed stream and another stream which is air you have two different exit stream one is the half gas where oxygen from air has been consumed and only the mixture of gases is leaving and you also have the another which is the product stream that contains acetic acid.

It has been told that the amount of acetic acid is produced would be 2 kilograms and it also told that the concentration of acetic acid cannot be higher than 12% indicating that the maximum concentration tolerated by the services 12% so that we will assume 12% acetic acid is present in the stream.

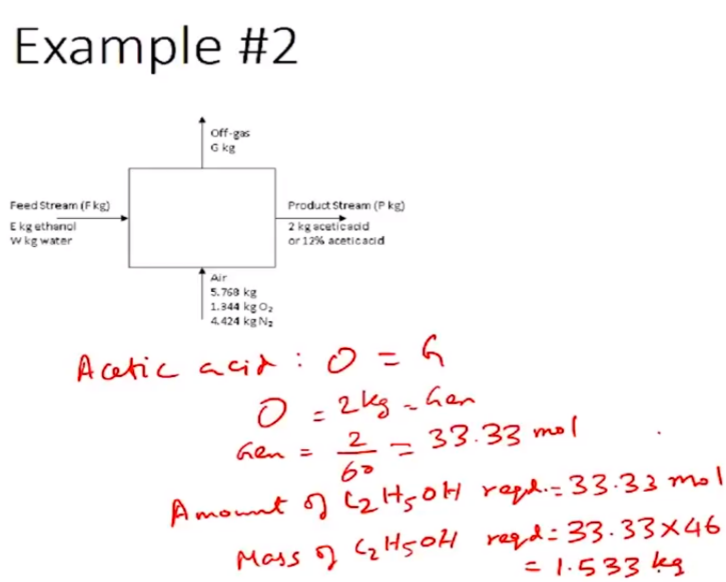
Why we assume this is in the second part of the problem we have been asked to calculate the minimum amount of water which is required for diluting the solution could get 12% if you want minimum amount of water which is used for dilution we would have to assume that the concentration of acetic acid would be 12%. If the concentration where to be lesser than that the amount of water used would be more than the minimum requirement.

So for this reason we will assume the concentration of acetic acid is in the product stream as 12% now for performing the calculation we need to know how much of nitrogen and oxygen are entering through the air stream. So we know that the composition of air is given as 79% nitrogen and 21% oxygen. So air contains 79% nitrogen and 21% oxygen so we have been told that 200 moles per hour air is fed.

So this 79 and 29% are the mole percentages so this implies 158 moles per hour of nitrogen and 42 moles per hour of oxygen is fed into the system. So this 158 moles per hour of nitrogen would be 158 times 28 grams of nitrogen per hour and 42 moles of oxygen would be 42 times 32 grams per hour of oxygen. So using this we can calculate the mass of nitrogen and as mass of nitrogen is 4.434 kilograms per hours and mass of oxygen is 1.343 kilograms per hour.

So the mass of air entering the system would be the summation of these two would give you 5.768 kilograms per hour.

(Refer Slide Time: 22:04)

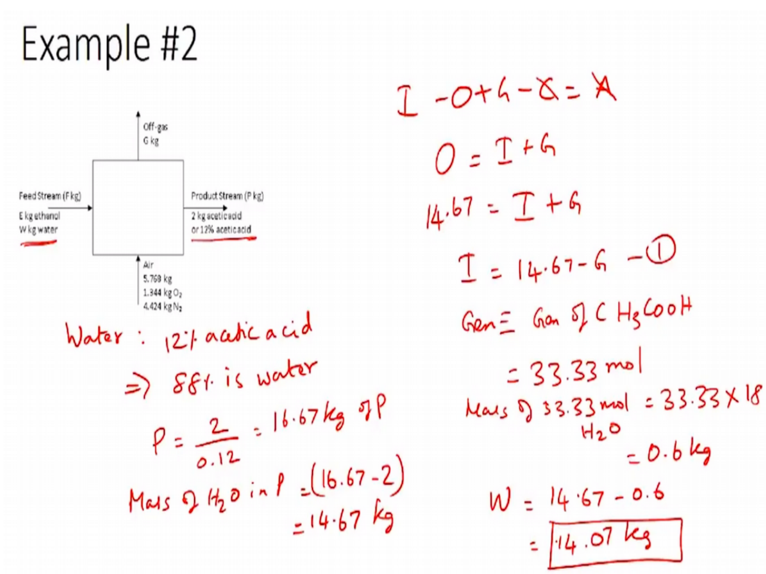


So now that we have calculated the composition of air we now have to move to the first part of the problem where we have been asked to calculate the minimum mass of ethanol required for producing 2 kilograms per hour acetic acid. So for this you will have to start with acetic acid balance so if we start with the acetic acid balance you would end up with output = generation + there is no input of acetic acid.

And obviously acetic acid is so not being consumed in this reaction and using accumulation to be 0 of a steady state process we end up with output equals generation which is 2 kilograms of acetic acid being produced. Now if this is the generation we can also calculate the number of moles of acetic acid which is generation so that we can use the stoichiometric. So generation in terms of moles for acetic acid would be the mass divided by molecular weight giving you 2 / 60 so conversion to moles will give you 33.33 moles.

So 33.33 moles of acetic acid is generated during this process based on the stoichiometric we know that 1 mole of ethanol which reacts forms one mole of acetic acid so to produce 33.33 moles of acetic acid the minimum amount of ethanol is required is also 33.33 moles. So amount of C2H5OH required is 33.33 moles so to calculate the mass of ethanol required you would multiply with molecular weight. So there by we get 33.33 times 46 giving you 1.533 kilograms.

(Refer Slide Time: 24:21)



Now we next part of the problem we have been asked to calculate the minimum amount of water that is required for diluting the acetic acid solution so that the percentage of acetic acid is not exceed 12%. So this we need to perform a material balance on water. So let us try and write a water balance equation for that we need to understand the composition of the product stream.

The product contains 12% acetic acid which means the rest 88% is water so the mass of the product stream P can be calculated as mass of acetic acid divided by the mass fraction of acetic acid giving you a value of 16.67 kilograms of P which is the acetic acid solution if 2 kilograms of 16.67 kilograms is acetic acid mass of water in the product stream would be 16.67 – 2 giving you 14.67 kilograms leaving through the product stream.

So we need to have 14.67 kilograms in product stream so that the water dilutes acetic acid to a 12% concentration. To get 14.67 kilograms of water in the product we would have to water which is supplied through the feed. In addition to the water which is fed you have water which is generated during the reaction if you have looked at the reaction the reaction scheme shows that ethanol forms acetic acid and water when it reacts with oxygen.

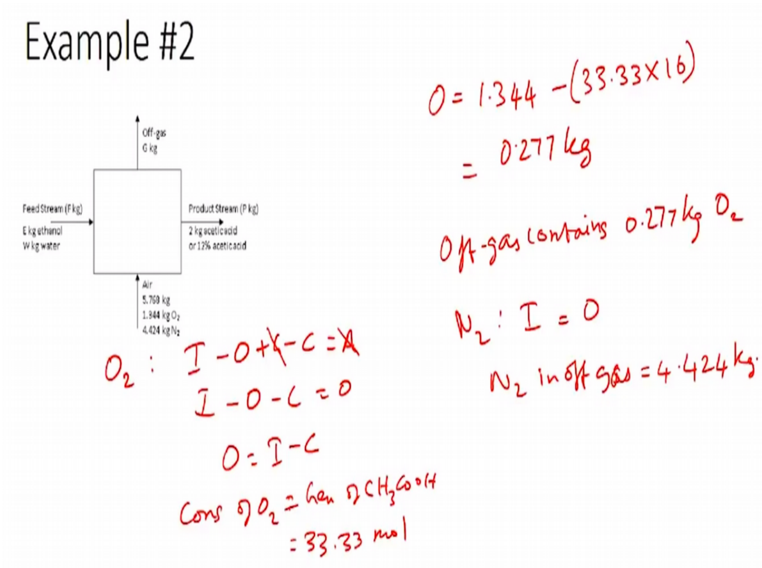
So we have water which is also generated so we can account for that while we are calculating the minimum amount of water that needs to be supplied for diluting the acetic acid solution. Let us write the balance equation for water it would look like input – output + generation – consumption = accumulation with accumulation going to 0 for steady state process water with the smart consumed in the reaction so consumption goes to 0 so you are left with input – output + generation = 0.

So we already know that output so we can output as input + generation and we know that the output is 14.67 kilograms input + generation so the amount of water which should be fed would be input is 14% - generation so we need to calculated the generation of water in this reaction what is the amount of water which should be generated.

If you looked at the stoichiometry you would have seen that for every mole of acetic acid produced 1 mole of water is also produced which means of water will be equal to generation of acetic acid. So thereby this is equal to 33.33 moles of water would have a mass of 0.33 moles could be equal to 33.33 times 18 giving you a mass of 0.6 kilograms.

So substituting back into this equations which is the balance equation for water you get the mass of water which is fed W = 14.67 – 0.6 giving you 14.07 kilograms. So we need to feed at least 14.07 kilograms of water to ensure that the product is diluted to have 12% acetic acid.

(Refer Slide Time: 28:52)



For the last part of the problem we have been asked the problem calculate the composition of gas which is leaving the system for that we need to write the balance for oxygen and nitrogen. So we know that 1.34 % of oxygen and 4.424 kilograms of nitrogen are entering into the system.

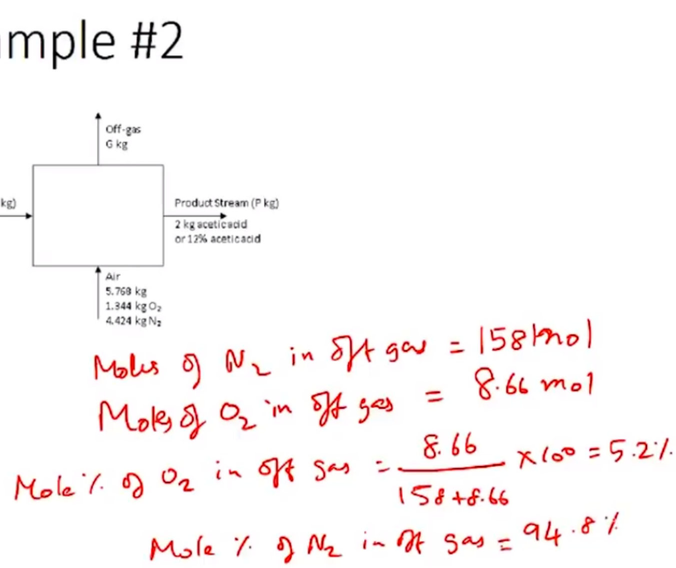
So let us write the oxygen balance to calculate how much oxygen have actually been consumed during this reaction. So oxygen balance would start from again input – output + generation - consumption = accumulation. So oxygen is not generated it is not accumulated at steady state conditions so giving you input – output – consumption = 0 so you are left with has input – consumption.

We know the mass of oxygen which is input we need to know the consumption of oxygen how do we calculate the consumption of oxygen using the stoichiometry we know that consumption of oxygen would be the same as the generation of acetic acid for every mole of oxygen consume one mole of acetic acid is generated which means 33.33 moles of oxygen has been consumed in the process where we have produced 33.33 moles of acetic acid.

So using this we can calculate the mass of oxygen leaving the system so mass of oxygen leaving the system out which is input which is 1.344 kilograms – consumption 33.33 moles converting this to mass to multiplying with molecular weight is 16 you would end up with so you would end up with mass oxygen of gas has 0.277 kilograms so off gas contains 0.277 kilograms of oxygen nitrogen does not take part in the reaction which means the nitrogen balance becomes very simple input = output.

So output of nitrogen in the off gas would be the same as the nitrogen which was fed which is 4.424 kilograms now that we have the masses of nitrogen and oxygen you would have to calculate the composition of nitrogen and oxygen so that we either calculate as mass fractions of mole fractions considering it is a gas the more appropriate way to calculate these things as mole fraction.

(Refer Slide Time: 31:59)



So what we can do for that is convert the mass of oxygen and nitrogen to moles of nitrogen and oxygen. So moles of nitrogen in half gas = moles of nitrogen in the half gas would be equal to 158 moles and moles of oxygen in half gas = 8.66 moles you can perform these conversions to confirm these numbers. So mole percentage of oxygen in half gas would be equal to 8.66 moles / 156 + 8.66 times 100 giving you a value of 5.2 percent.

So the rest would be nitrogen so you have mole percentage of nitrogen in half gas as 94.8 % so this gives composition of the half gas which is leaving the system. So right now we have actually performed two different problems to solve material balance equations for processes with reaction. One of the common things with both the systems where the reactions equation where given here.

In the next class we will perform one simple example problem where the stoichiometry is not given in the traditional we will look at a problem which as clinical applications that provided the values which are related to stoichiometric in a more common in an industry or in an application rather than seen in a chemistry class meet you all next week thank you.