Material and Energy Balances

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

Module No # 03
Lecture No # 15
Material Balance Calculations for Single Units With A Single Reaction – Part 3

Welcome back for the problems on material balances for systems which have in the multiple reaction in the earlier lecture we saw examples where the reactions are happening in parallel and we tried 3 different techniques for solving these material balances problems namely the molecular species balance, atomic species balance and the extent of reaction methods.

I has asked to try the problem using molecular species balances to see whether you fully understood the techniques which we have discussed I hope we have done the exercise now let us move on to the example problem where reaction as are happening in series.

(Refer Slide Time: 00:56)

Example #3: Reactions in series

- Formaldehyde (HCHO) is produced industrially by the catalytic oxidation of methanol (CH_3OH) according to the following reaction:

  $$CH_3OH + 0.5O_2 \rightarrow HCHO + H_2O$$

  Unfortunately, under the conditions used to produce formaldehyde at a profitable rate, a significant portion of the formaldehyde reacts with oxygen to produce CO and H_2O, that is,

  $$HCHO + 0.5O_2 \rightarrow CO + H_2O$$

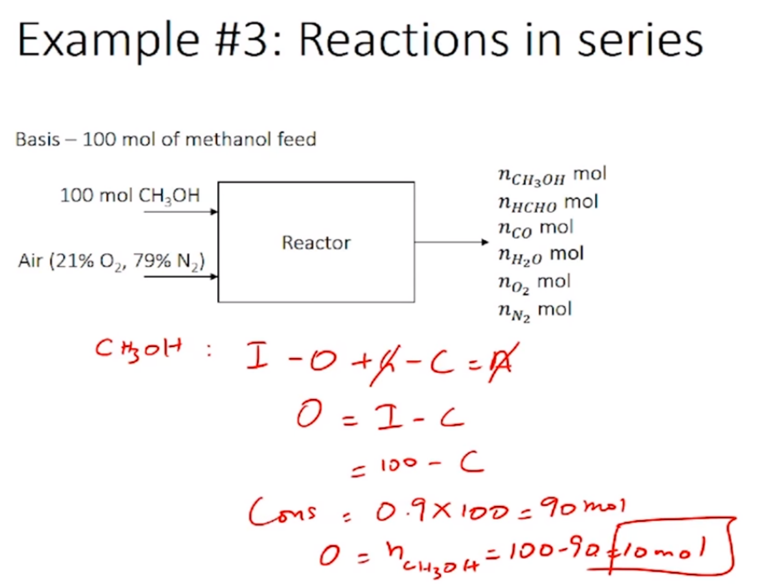
  Assume that methanol and twice the stoichiometric amount of air needed for complete conversion of the CH_3OH to the desired products are fed to the reactor. Also assume that 90% conversion of the methanol results, and that a 75% yield of formaldehyde occurs based on the theoretical production of HCHO by reaction 1. Determine the composition of the product gas leaving the reactor.

Let us look at these example problem formaldehyde is produced industrially by catalytic oxidation of methanol according to the following reaction methanol reacts with oxygen to form formaldehyde and water. Unfortunately under the condition used to produce formaldehyde at a profitable rate a significant portion of formaldehyde react with oxygen to produce carbon monoxide and water in the given reaction.

Assume that methanol and twice the stoichiometric amount of air needed for complete conversion of methanol to the desire product are fed to the reactor also assume that 90% conversion of methanol results and that 75% yield of formaldehyde occurs based on theoretical production of formaldehyde by reaction 1 you are asked to determine the composition of product gas leaving the reactor.

As the product gas stream is leaving in the gas phase you will assume the basis in terms of moles thereby we can get the final values in moles and perform calculations in the simpler way for this reason we will assume the basis to be 100 moles of methanol fed.

(Refer Slide Time: 02:07)



Based on the basis and the information given to the problem we have 100 moles of ethanol entering the reactor along with air which would contain 21% oxygen and 79% nitrogen which reacts in the reactor to form different component. So you have the unreacted methanol leaving and you also have formaldehyde leaving carbon monoxide water oxygen and nitrogen which are leaving the system.

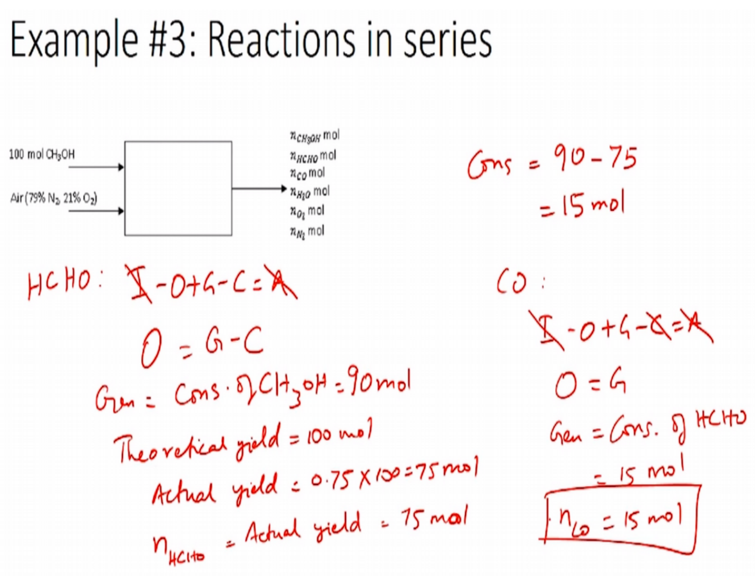
Now that we have the flow chart to describe the process let us try to solve this problem as we have used the basis in terms of moles we cannot start with equation because total moles of system is not conserved during the reaction. So instead we will start with the component balances. The first component balance for which we write the balance equation would be methanol.

So let us start with methanol balance CH3OH so the equation would be input – output + generation – consumption = accumulation. So where which of these terms will goes to 0 at steady state accumulation goes to 0 methanol is a reactant and it is not being generated so generation terms goes to 0 so we are left with input output and consumption so the output term which we need to calculate would be input – consumption.

Based on the basis we used we know that the input of methanol is 100 moles we need to know not he consumption of methanol. We have told that the consumption of methanol the conversion of methanol is 90% so using that the consumption can be calculated as 0.9 which is the conversion times 100 giving you the total conversion the total consumption as 90 moles.

So therefore the methanol which is leaving the system would be O which equals to output this NCH3OH moles which is 100 – 90 giving you 10 moles so 10 moles of methanol is leaving the system.

(Refer Slide Time: 04:21)



The second component we can write the balance equation for is formaldehyde so again we start with input – output + generation – consumption = accumulation at steady state accumulation goes to 0 methanol sorry formaldehyde here actually is a product in the first reaction and it is a reactant in the second reactant which means within the reactor it is being generated and consumed however there is no input of formaldehyde for the system.

So input goes to 0 so the output term we have would be equal to generation – consumption so how do we calculate the consumption the generation term. So the generation of formaldehyde would be equal to the consumption of methanol based on the stoichiometric so generation is equal to consumption of methanol giving us the value of 90 moles however we have also been told that the actual yield of formaldehyde is 75% of the theoretical yield of formaldehyde based on methanol fed.

So this means you would have to assume the theoretical yield to be the amount of formaldehyde which would have been produced had the methanol being fully converted only to formaldehyde. So this would results in 100 moles of formaldehyde being formed we have been told that the actual yield is 75% of the theoretical yield there by what we observed as the output would be 75 moles of ethanol sorry formaldehyde.

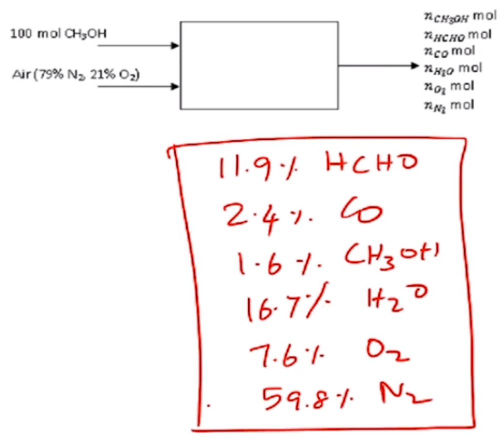
So as I said theoretical yield of formaldehyde would have been 100 moles so actual yield was 75% of that giving you only 75 moles. So the output NHCHO would be basically the actual yield giving you 75 moles. From here we can calculate the consumption term as generation – output generation being 90 and output being 75 giving you 15 moles so this now tells you how much of formaldehyde is consumed by the second reaction.

So we can now write a carbon monoxide balance the carbon monoxide balance would again start from input – output + generation – consumption = accumulation steady state accumulation goes to 0 we would have any consumption because carbon monoxide is only being produced there is no input for carbon monoxide thereby the output = generation of carbon monoxide. So based on the stoichiometric we know that generation of carbon monoxide will be equal to the consumption of formaldehyde in the reaction 2.

So general here would be equal to consumption of formaldehyde thereby the generation term is 15 moles. So the output for carbon monoxide NCO would be equal to 15 moles.

(Refer Slide Time: 08:05)

Example #3: Reactions in series



The next component for which we can write a balanced equation would be water. So let us write the water balance again as usual start with general balance equation which is input – output + generation – consumption = accumulation. So water is not consumed in the reactions and at steady state there is no accumulation also and there is no input of water giving you output = generation.

However water is generated by both the reactions reaction 1 and reaction 2 so for this reason we would have the output for water would be equal to generation of water in reaction 1 + generation of water in reaction 2. So generation of water in reaction 1 would be equal to consumption of methanol in reaction 1 this is based on stoichiometry. So this would be equal to consumption of methanol in reaction 1.

So we know that the consumption of methanol in reaction a is 90 moles so generation of water reaction 1 will also be equal to 90 moles. Similarly generation of water in reaction 2 will be equal to consumption of formaldehyde in reaction 2. We know that consumption of formaldehyde in reaction 2 is 15 moles so thereby giving generation of water in reaction 2 to in 15 moles.

So the output is basically the summation of these two so NH2O = 90 + 15 giving us 105 moles. So now we can write a balance equation for oxygen balance would be again we start off with the general balance as input – output + generation – consumption = accumulation at steady state accumulation goes to 0 oxygen is only consumed it is not being produced. So generation goes to 0 we have input oxygen in the form of air and we have output oxygen which is the unreacted air leaving the system.

So for this reaction we would have output = input – consumption we can calculate the amount of oxygen which is supplied in the system based on the information given to us in the problem the problem statement tells us that air is supplied at twice the stoichiometric amount as what is required for complete conversion of methanol for desired products which are fed to the reactor. So now based on this information we can calculate the amount of oxygen fed as follows.

Oxygen supplied which is the input = 2 times stoichiometric requirement in reaction 1 so from the reaction stoichiometric we know that every mole of a methanol required half a mole of oxygen for the reaction which means when you are supplying it in the rate of 2 times so we have two times 0.5 which is the stoichiometric amount twice the stoichiometric amount times 100 moles which is the number of moles of methanol which is being fed to the system.

We actually are supplying 100 moles of oxygen to the system so substituting the value back here we get output = 100 moles – consumption. Now let us look at what the consumption would be so consumption of oxygen in reaction 1 would be half the reaction of formaldehyde or half the reaction of consumption of methanol. So this would be half times consumption of methanol and consumption of oxygen in reaction 2 would be half the consumption of formaldehyde in the reaction.

So now having this information the total consumption of oxygen would be 0.5 times 90 + 0.5 times 15 giving us the total value of 52.5 moles. So now the number of moles of oxygen leaving the system NO2 would be equal to input – consumption input is 100 moles and consumption is 52.5 moles so NO2 = 47.5 moles. So the last component for which we need to write the balance equations would be nitrogen.

Nitrogen is a non-reacting component in the system so you would have input = output so we can write the nitrogen balance as input =output giving raise to calculation for input alone. So based on the information we have for oxygen we can calculate the amount of nitrogen so we know that

100 moles of oxygen is fed so this means this 100 moles constitutes 21% of air so rest 79% is nitrogen.

So based on that we can calculate input of nitrogen as 100 divided by 0.2 times 0.79 which gives us the value of 376.2 moles. So N nitrogen which is leaving the system would be equal to the system which is 376.2 moles now that we have the number of moles for each of the system in the components in the system we have to now calculate the mole fractions follows total number of moles in product gas would be total equals NCH3OH + NHCHO + NCO + NH2O + NO2 + NN2.

So adding all these values 10 + 75 + 15 + 105 + 47.5 + 376.2 giving you the total number of moles as 628.7 moles using the individual moles for each of the components and the total moles we can calculate the mole fraction or mole percentage of each of the component in product stream. So the composition of the product stream using that would be 11.9% formaldehyde 2.4% carbon monoxide 1.6% methanol 16.7% water 7.6% oxygen and 59.8% nitrogen.

So this gives you the molar composition of the product gas which we have obtained through this process with this we come to the conclusion of the example problems where we use single unit processes with multiple reactions in the subsequent lectures we will look at multi-unit processes where reaction or reactor is one of the units and we have other units so just like we solved for multi-unit processes without reactions the critical aspect would be choosing the correct system.

So we will move on to that in the next lecture thank you.