Material and Energy Balances
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Module No # 03
Lecture No # 13
Material Balance Calculations For Single Units With A Single Reaction – Part 1

Hello everybody welcome to today's lecture on material balance calculation for single unit with multiple reactions. In the last few lectures we have performed some example problems where we did material balances for reactive process in those systems we had only a single reaction taking part inside the reactant. Here we are going to look at reactions which are happening either in parallel or in series and try to use the same principles which we learnt and the terminologies associated with multiple reaction to solve for the flow rates and conversions.

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Example #1: Parallel reactions

- Methane is burned with air in a continuous steady-state combustion reactor to yield a mixture of carbon monoxide, carbon dioxide, and water. The reactions taking place are,

$$CH_4 + 1.5O_2 \rightarrow CO + 2H_2O$$

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

The feed to the reactor contains 7.80% CH_4, 19.4% O_2 and 72.8% N_2. The percentage conversion of methane is 90% and the gas leaving the reactor contains 8 mol CO_2/mol CO. Calculate the molar composition of the product stream using molecular species balances and atomic species balances.

Let us start with the first example problem methane which is burnt with air in a continuous steady state in a combustion reactor to yield a mixture of carbon mono oxide, carbon dioxide and water the reaction which are taking place are given as methane + oxygen forming carbon monoxide and water and methane + oxygen forming carbon dioxide and water the feed to the reactor contains 7.8% methane 19.4 % oxygen and 72.8% nitrogen.

The percentage conversion of methane is 90% and the gas leaving the reactor contains 8 moles of carbon dioxide per mole of carbon monoxide. You are asked to calculate molar composition of the composite stream using both molecular species balances and atomic species balances. Let us now try to solve this problem if you look at the problem you see that no flow rates has been given.

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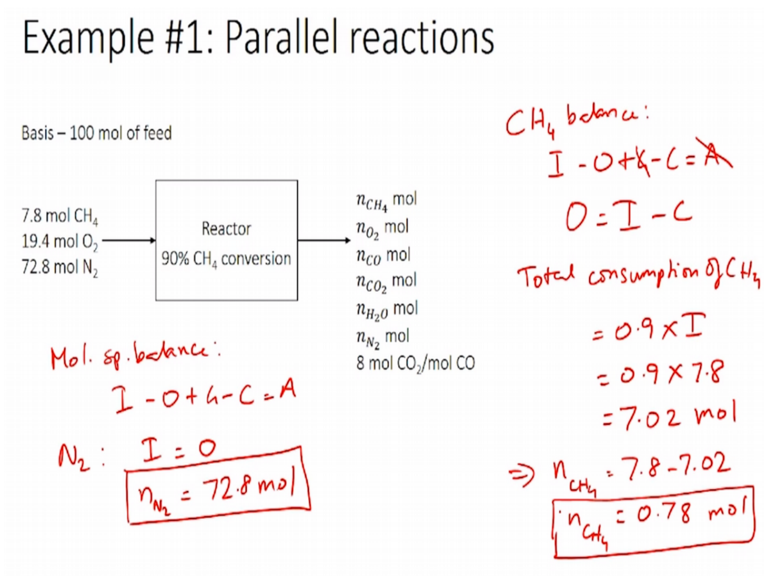

So we can use the convenient number as the basis so here I have assumed a basis of 100 moles of feed as we have the moles percentages for the feed stream which is coming in we can calculate the composition of the feed stream as 7.8 moles of methane 19.4 moles of oxygen and 72.8 moles of nitrogen entering the reactor where 90% of methane is converted to form product stream which contains unreacted methane and oxygen and also contains cordon dioxide, carbon monoxide, water vapor and nitrogen leaving the system.

It has also being given that the ratio of carbon di oxide to carbon mono oxide is 8 moles is to 1 mole. So this is the selectivity or the reaction so now that we have the selectivity and the composition of the feed stream and also the conversion let us try to perform the material balance calculation to get the number of moles in each of the component in the product stream and then calculate the molar composition of the product stream.

So the problem requires us to perform both molecular species balances and atomic species balances. Let us first start with molecular species balances so the molecular species balances can be written as follows you have input – output + generation – consumption = accumulation. For non-reactive components generation and consumption go to 0 and steady state accumulation would go to 0.

So let us start with nitrogen so in case of nitrogen it is a non-reactive component. So generation and consumption will be 0 our steady state accumulation will also be equal to 0 giving you input = output so the input moles of nitrogen is known as 72.8 moles of nitrogen so based on that NN2 which is the number of moles leaving through the product stream would also be equal to 72.8 moles.

So this gives you the first information now we can write the balance equation for the other composition. Let us start with methane balance so methane balance would be again input – output + generation – consumption = accumulation no accumulation at steady state methane is a reactant which means the there is no generation of methane. So the equation for output is input – consumption input is already known so we just need to calculate the consumption.

So methane can technically been consumed by both the reaction so reaction 1 and 2 both consume methane and it as been told the total consumption of methane is 90% which is the conversion of the methane. So total consumption for methane would be 0.9 times input which is 0.9 times 7.8 moles giving you a total consumption of 7.02 moles. So thereby we can calculate the output which is NCH4 as 7.8 – 7.02 giving you 0.78 moles of methane leaving the system.

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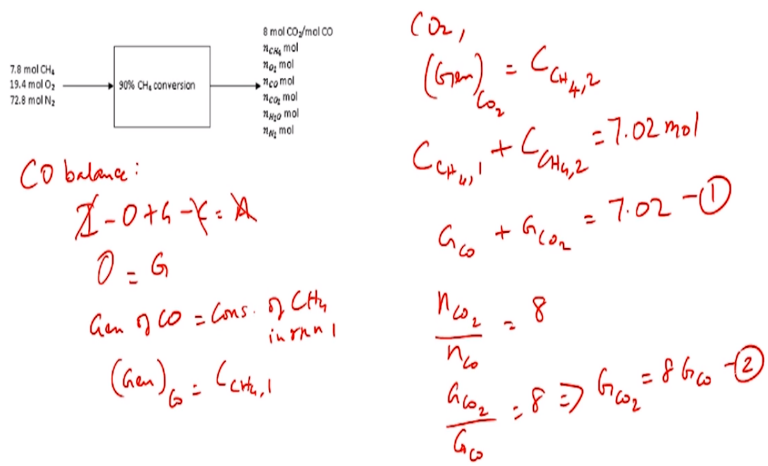
Example #1: Parallel reactions



So we have now calculated the number of moles of nitrogen and methane let us start writing the balance for carbon monoxide CO balance again input – output + generation – consumption = accumulation. So carbon monoxide is product which means there is no consumption and there is only generation at steady state there is not accumulation also so your output term becomes input + generation.

So our carbon monoxide is not entering the system also output is actually = only generation so to calculate generation of carbon di oxide sorry generation of carbon monoxide we need to know how much of methane is entering into the first reaction and how much of methane is entering into the second reaction. So let us call the consumption of methane by the first reaction as CH41 so generation of carbon monoxide.

So generation of carbon monoxide would be equal to consumption of methane in reaction 1 based on stoichiometric so this generation term for carbon monoxide = consumption of methane in the first reaction. Similarly for carbon dioxide the generation term for carbon dioxide would be equal to consumption of methane in the second reaction now we already know that the total consumption of methane is 7.02 moles which means consumption of methane in the first reaction + consumption of methane in second reaction = 7.02 moles.

So substituting the generation terms for carbon monoxide and carbon dioxide there we would have GCO + GCO2 which are the generation terms equal to 7.02. So this can be equation 1 another information which has been given to us is the ratio of carbon dioxide and carbon monoxide in the output streams which is NCO2 divided by NCO = 8 so we already know from the balance equation that the number of carbon dioxide would leaving the system would be equal to amount of carbon dioxide generate it.

And similarly number of carbon monoxide moles leaving would be equal to the number of carbon monoxide moles that are generated. So substituting the generation term here again you would have GCO2 divided by GCO would be equal to 8 giving you a equation for GCO2 = 8GCO so this is the second equation.

So now that we have two equations and two unknowns we solve or the number of moles of the carbon dioxide and carbon monoxide that is generated which would also be equal to the number of moles of carbon monoxide and carbon dioxide that is actually leaving the system.

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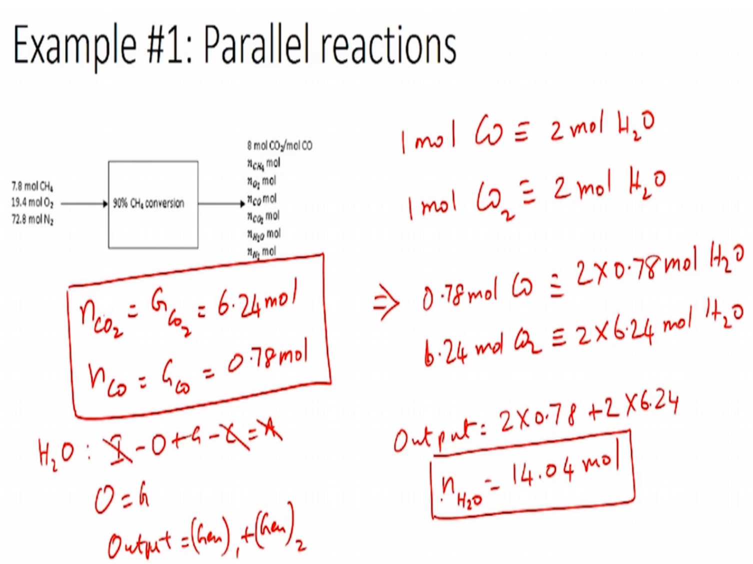

By solving these two equations we get NCO2 which is equal to generation of CO2 as 6.24 moles and NCO which is equal to generation of carbon monoxide again which is equal to 0.78 moles. So this gives us the information about the carbon monoxide and carbon monoxide leaving the system. So now we have calculated the number of moles methane leaving the system number of moles carbon monoxide leaving the system number of moles of carbon dioxide leaving the system and number of moles of nitrogen leaving the system.

We still need to calculate the number of moles of water and oxygen which are leaving the system so let us write a balance for water we start again with input – output + generation – consumption = accumulation so now accumulation at steady state water is a product which means a consumption there is also water not entering the reactor which means your generation = output. However in this case water is generated by both the reaction.

So your total output which you get would be equal to generation from reaction + generation from reaction 2. So how do we calculate the generation for each of these reactions from the stoichiometric we know that for every mole of CO generated in reaction 1 two moles of water is generated similarly for every mole of CO2 generated in reaction 2 you have two moles of water generated.

Therefore you know that 0.78 moles of CO generated implies that 0.2 times moles of water generated by reaction 1 and 6.24 moles of CO2 generated by reaction 2 implies 2 times 6.24 moles of water generated by reaction 2. So the total output would be equal to the generation of these two terms which is 2 times 0.78 + 2 times 6.24 giving you a value of 14.04 moles so this would be the number of moles of water present in the product so we still need to calculate the number moles of oxygen leaving the stream.

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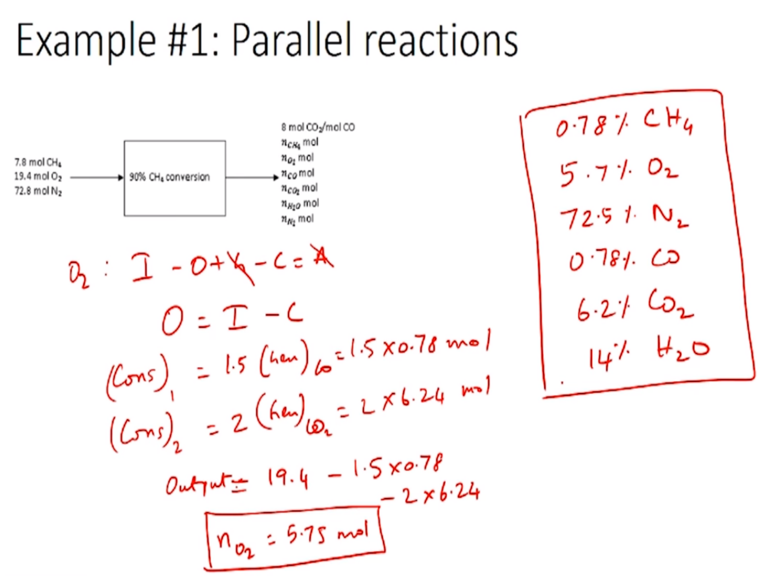

So let us write the oxygen balance start with input – output + generation – consumption = accumulation. Oxygen being a reactants is not generated it not as not accumulation under steady state conditions giving you input – output + generation – consumption = 0 so your output = input – consumption oxygen is consumed in both the reaction so consumption in reaction 1 would be what?

So we know that for every mole of carbon dioxide produced you have two moles of oxygen which is consumed. From the stoichiometric you know that for every mole of carbon dioxide produced you have two moles of oxygen consumed and for every mole of carbon monoxide consumed you have 1.5 moles of oxygen which is used.

So using that we can calculate the consumption of oxygen in the first reaction as 1.5 times the generation of carbon monoxide which would be 1.5 times 0.78 moles and consumption of oxygen in the second reaction would be equal to two times generation of carbon dioxide which is two times 6.24 moles. So the total output of oxygen would be input which is 19.4 moles of oxygen – 1.5 times 0.78 which is the consumption from reaction 1 – 2 times 6.24 which is the consumption by reactant 2 giving you the final output as NO2 = 5.75 moles.

With that we have all the components which are present in the product stream we know the moles of each of the components the summation of all these moles will give us the total moles of the system using that we can calculate the product composition. So the product composition would be 0.78 % methane 5.7 % oxygen 72.5 % nitrogen 0.78% carbon monoxide 6.2% carbon dioxide and 14% water vapor.

So this is the product composition given in the terms of molar percentages this is how we would go about solving this problem using molar species balances. Now let us see if we can solve the same problem using atomic species balance and let us compare the answers and see whether we get the same answer you can also try to see which of the techniques is simpler for you and try to adopt of these techniques for your calculations.

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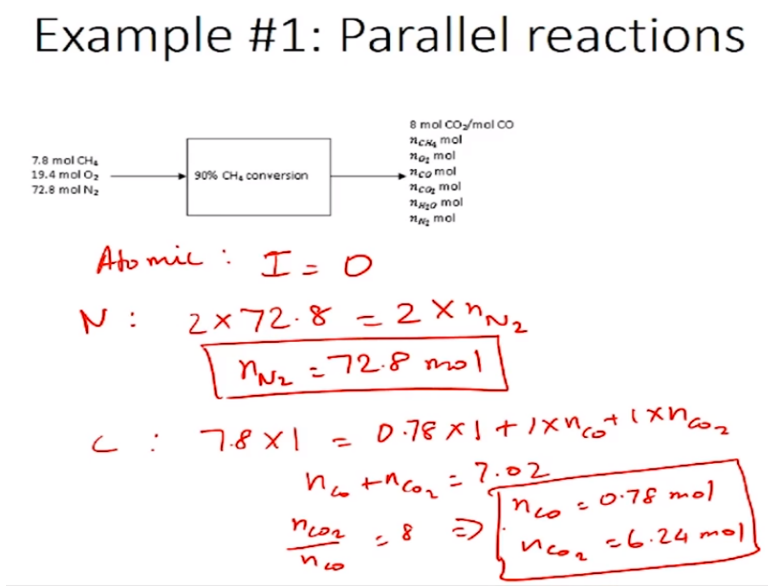

Now that we are considering atomic species balances we need to understand generation and consumption terms go to 0. Atoms cannot be created or destroyed so generation and consumption are 0 at steady state accumulation is also 0 so all atomic species balance we would have would form the would follow the form input = output let us start writing the atomic species balances for nitrogen.

So nitrogen balance would be two atoms of nitrogen entering the each molecule of N2 there by giving an input of two times 72.8 and the output would also be 2 times NN2 + you have two atoms of nitrogen leaving in the form of nitrogen leaving in the molecules so your NN2 = 72.8 moles. So now we can write a carbon balance we when we write a carbon balance we need to know how much carbon is entering which is in the form of methane.

So you have 7.8 moles of carbon entering and there is only one atom of carbon in methane so 7.8 times is to 1 = number of atoms of carbon which is leaving the system would be 0.78 times 1 in the form of methane so we know this because we know it is 90% conversion of methane so thereby only 0.78 moles of methane leaving the system and we have 1 atom of carbon in carbon dioxide and one atom of carbon in carbon monoxide.

So we write it as 1 times NCO + 1 times NCO2 so this gives us an equation of NCO + NCO2 is equal to 7.02. So already know that NCO2 divided by NCO = 8 this information has been given in terms of selectivity so using that in the first equation we can calculate NCO and NCO2 as 0.78

moles and 6.24 moles. So this gives us the carbon monoxide and carbon dioxide in the product stream.

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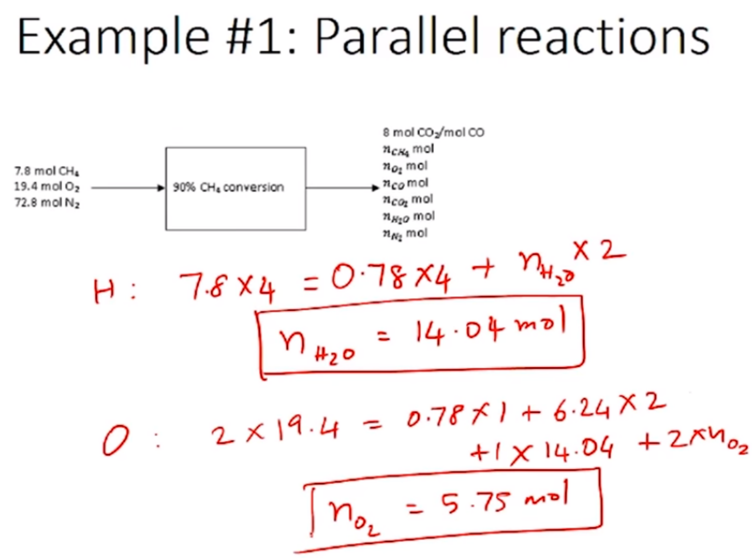

We can now write the balance equation for hydrogen and oxygen to perform this calculation hydrogen balance we have four atoms of hydrogen entering per molecule of methane so atomic balance for hydrogen would be 7.8 times 4 which is input = 0.78 times 4 which is the number of atoms of hydrogen leaving through methane + NH2O times 2.

So using this we can calculate NH2O as 14.04 moles and finally we can write the oxygen balance which would be 2 atoms of oxygen per molecule of oxygen entering which is 19.4 times 2 is equal to 0.78 times 1which is the number of moles of carbon monoxide which is leaving the system + 2 times the number of moles of carbon dioxide leaving the system which is 6.24 + 1 times the number of moles of water vapor leaving the system which is 1 times 14.04 + 2 times number of molecules of oxygen leaving the system giving you NO2 = 5.75 moles.

So again we have been able to calculate all the terms which we have looked for so if were to compare the values which we got through molecular species balance and atomic species balance they would all be the same validating that the technique we used and the final answers we arrived are accurate so we can again calculate the molar percentage using these values to get the same values as we got using molecular species balance.

So with that we will come to the conclusion for today's lecture we will continue with more example problems where reaction happen in parallel and series for us to get more clarity on how to solve such problems thank you.