Material and Energy Balances

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Module No # 03
Lecture No # 14
Material Balance Calculations for Single Units With A Single Reaction – Part 2

Welcome back to the lectures on material balance calculation for single unit systems with multiple reaction in the last lecture we looked at molecular species balances and atomic species balances for problem which had two reactions happening in parallel. So let us try a different technique for two reactions happening in parallel today.

So this example problem again as two reaction happening in parallel however the technique which we use would be different from the molecular species balance and atomic species balance which we use the technique is going to use is called extent of reaction technique.

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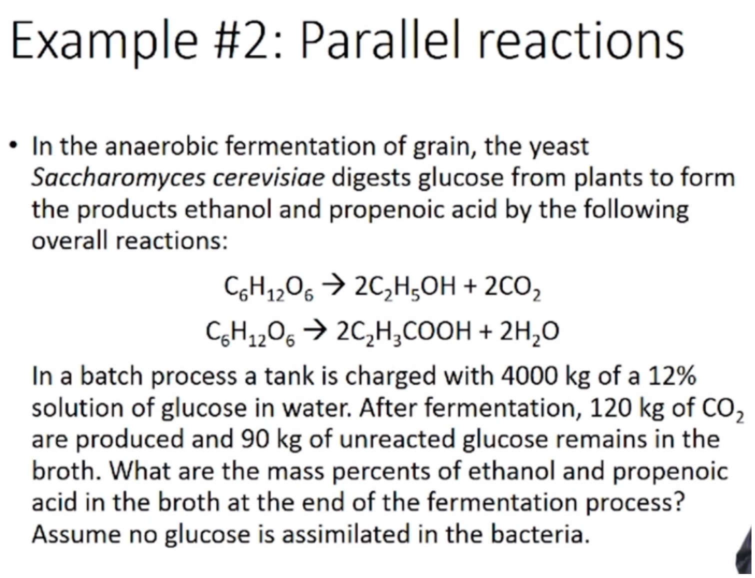

So let us go about reading the problem statement in the anaerobic fermentation of grain the yeast saccharomyces cerevisiea digests glucose from plants to form the products ethanol and propionic acid by the following overall reactions in a batch process a tank is charged with 4000 kilograms of 12% solution of glucose in water after fermentation 120 kilograms of carbon dioxide is produced and 90 kilograms of unreacted glucose remains in the broth.

What are the mass percent's of ethanol and propenoic acid in the broth at the end of the fermentation process. You can assume that no glucose is assimilated in the bacteria so based on the information given you can assume the steady state because there is no accumulation happening.

So we will go about solving this problem so as I mentioned we will try to a use a technique called extent of reaction technique we have already defined what the extent of reaction is you will try to apply that for performing this material balance calculation. To start the problem we identify that 4000 kilogram of solution is present initially in the reactor.

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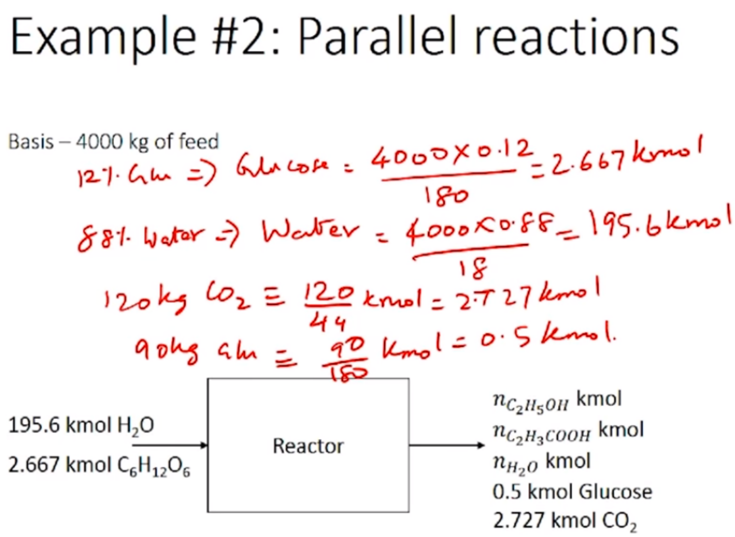

So the basis would be 4000 kilograms of feed now that we have the feed in mass we will have to identify how much of it is glucose and what is the amount of water you would have need to know the number of moles of glucose and water which is present so that we can use the stoichiometric effectively.

So let us first identify what information we have we have been told that 12% glucose solution is fed this implies that amount of glucose in the feed would be 4000 times 0.12 and converting this mass to moles we divided by the molecular weight which would be 180 kilograms per kilo mole giving you a value of 2.667 kilo moles. So the rest 88% is water this implies that the amount of water present in the feed would be 4000 times 0.88 divided by 18 which is the molecular weight of water to give the total number of moles as 195.6 kilo moles.

In addition to this we have also been told that the final product contains 90% kilograms of glucose and 120% kilograms of carbon dioxide. So we convert these masses to moles also 120 kilograms of carbon dioxide basically would be 120 divided by 44 moles 44 kilo moles of carbon dioxide which is 2.727 kilo moles and you have glucose which is 90 kilograms of glucose forming 90 divided by 180 kilo moles which is 0.5 kilo moles of glucose.

So let us now draw the draw the flow chart for the process the process would look like this we have 195.6 kilograms of water and 2.66 kilo moles of glucose entering the system where it gets reacted to form ethanol, proponioc acid, water and you have 0.5 kilo moles of unreacted glucose remaining and you have also have 2.727 kilo moles of carbon dioxide which is produced. With this information let us start solving the material balance problem.

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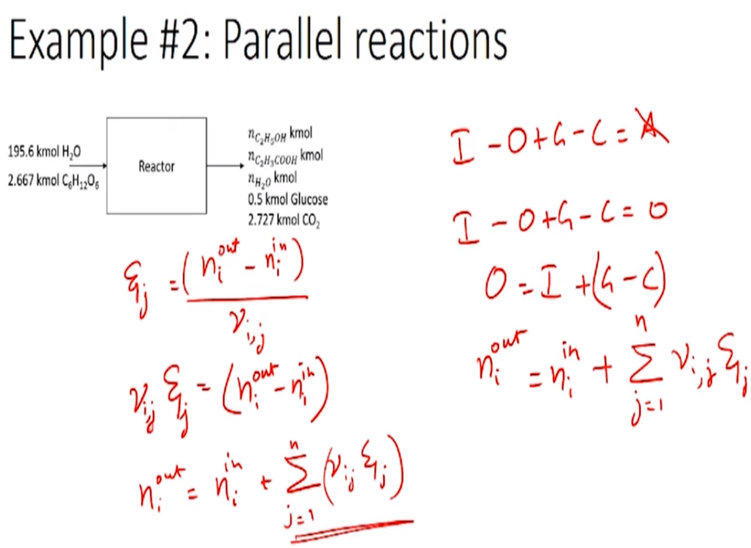

As I mentioned when we start this lecture we are going to use the technique called extent of reaction technique. We have already defined what an extent of reaction is extent of reaction for a reaction J is given as NI out – NI in so it could either for fine and in or initial divided by the stoichiometric coefficient of that particular reactant in the reaction J. So this is basically a representation of the change in the number of moles of a particular component during the reaction divided by the stoichiometric coefficient of that particular reaction.

So from this equation we understand that the product of stoichiometric coefficient of a component in the reaction J times the extent of reaction J for reaction J would basically give us N out – N in for a particular component which is basically the change in the number moles of a particular component this could either be generation or consumption because of this under steady state condition using extent of reaction we can write the balance equation as follows.

NI out would be equal to NI in + signo of J = 1 to N NuIJ extent of reaction for J how did I write this equation. So what we have is input – output – generation – consumption = accumulation which is the general balance equation, At steady state the accumulation is giving us the input - output – generation – consumption = 0 so input is basically sorry so output is basically equal to input + generation – consumption this term generation – consumption represents the change in the number of moles due to reaction.

So that can be represented as sigma of Mu IJ for the extent of reaction J and when we do this what we have is accounting for the number of moles for each component being consumed or generated for each of the reaction which is taking place and for finding us reaction of summation of all that we get the total change in the number of moles in the particular component in the process.

So thereby we write this out as NI out IN as NI in and that is the input and you have the generation – consumption which is represented by the summation of all the reactions stoichiometric coefficient of the component for that particular reaction times the extent of reaction for the particular reaction. So using this particular equation let us try and solve the material balance problem in front of us.

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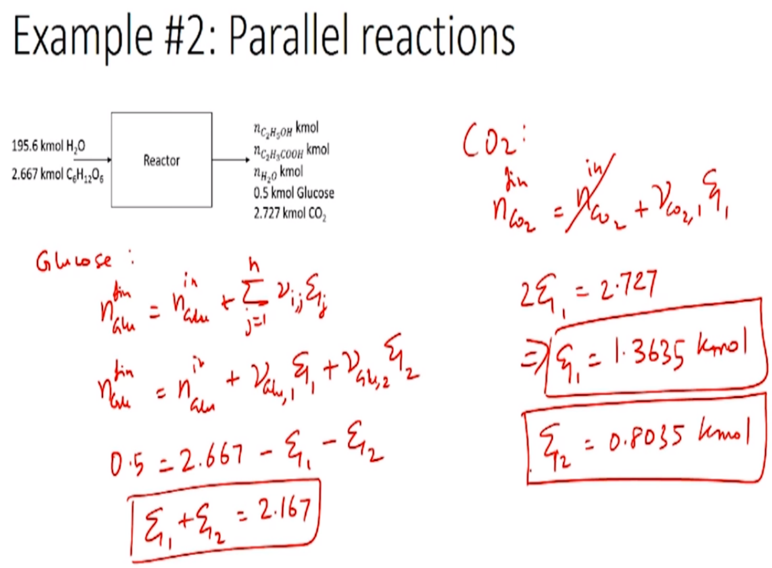

For this reason we will start with glucose where we know the amount of glucose entering and amount of glucose leaving and carbon dioxide where we know that no carbon dioxide is entering the system and we have the condition of how much carbon dioxide is present at the condition. So using that let us start with glucose balance the glucose balance would look like this you have glucose final would be equal to glucose initial + sigma of J = 1 to N Mu IJ stoichiometric coefficient times extent of reaction for J.

Glucose actually take part in both the reaction which means this equation becomes N glucose final = N glucose initial + the stoichiometric coefficient of glucose in the first times the extent of reaction for first reaction + the stoichiometric coefficient of glucose in second reaction in the extent of reaction for the second reaction. The stoichiometric coefficient of glucose in both the reaction is 1 and we know the number of moles of glucose in the final condition in the initial condition.

So looking at the data given in the problem we know the number of moles of glucose which is present in the initial condition and the number of moles of glucose is present in the final condition we also know that the stoichiometric coefficient for glucose in both the reaction is 1. However glucose is a reactant which means the stoichiometric coefficient would be written as negative 1 to account for the glucose being consumed instead of being generated.

Taking that into account the balance equation would look like 0.5 equals 2.667 – extent of reaction for reaction 1 and extent of second reaction giving you the summation of extent of reactions as 2.167 so this is 1 equation. Similarly we can write a balance equation for carbon dioxide. Carbon dioxide takes part only in the first reaction there is no carbon dioxide involved in second reaction for this reason the equations becomes simpler.

You have N carbon dioxide final equals N carbon dioxide initial + stoichiometric coefficient of carbon dioxide in the first reaction times the extent of reaction for the first reaction as there is no carbon dioxide in the initial condition you end up with the stoichiometric coefficient of carbon dioxide times the extent for reaction for carbon dioxide in the first reaction is equal to the amount of carbon dioxide in the final condition.

So the stoichiometric coefficient of carbon dioxide is 2 the carbon dioxide is product which means the stoichiometric coefficient will be written as a positive to which is two times extent of reaction for 1 would be equal to 2.727 giving you the extent of reaction for the first reaction as 1.3635 kilo moles. So substituting this back into the first equation we can get the extent of reaction for the second reaction as 0.8035 kilo moles.

Now that we have calculated the extent of reaction for 1 and 2 we can calculate the number of moles in the final condition for all the reactants and products which are taking part in the reaction for that we could write component balances for the individual components.

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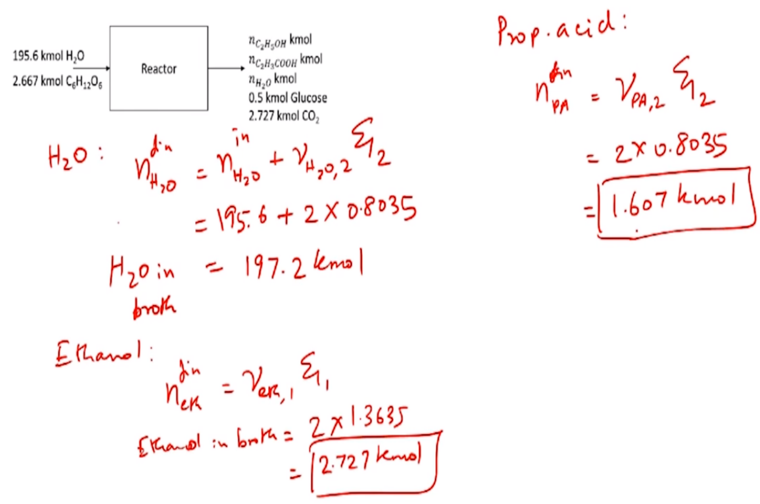
Example #2: Parallel reactions



Let us start with water balance so the water balance could be N water final = N water initial + stoichiometric coefficient of water in the second reaction times the extent of reaction for the second reaction water is not taking part in the first reaction and it is being produced in the second reaction for this reason we have used only the stoichiometric coefficient of water in the second reaction and the extent of reaction for second reaction.

So the initial amount of water is 195.6 and the stoichiometric coefficient of water is 2 times 0.8035 giving you the total amount in the final broth is water in broth would be 197.2 kilo moles and we can write the ethanol balance followed by this the ethanol balance would be again the same thing we have ethanol final we do not have ethanol entering the system in the initial condition and ethanol is being produced only in the first reaction.

So this becomes stoichiometric coefficient of ethanol in the first times extent of times reaction for the first reaction so there by ethanol in the broth is equal to 2 times the extent of reaction for the first reaction which is 1.3635 giving you the value of 2.727 kilo moles. So finally will have perform the balances for propoinoic acid so for propionic acid we do not have any propionic acid entering using at the initial condition and we have only propinioc acid being produced by the second reaction.

So propionic acid in the final condition would be equal to stoichiometric coefficient of propionic acid in the second reaction in the extent of reaction for the second reaction which is 2 times

0.8035 giving you the value of 1.607 kilo moles with this we have the number of moles of the each of the component present in the final broth. Now we need calculate the composition of the final broth.

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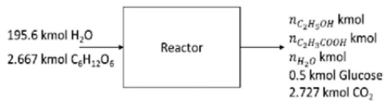
Example #2: Parallel reactions



Component	Amount (kmol)	MW (kg/kmol)	Mass (kg)	Mass percentage
Ethanol	2.727	46	125.44	3.14
Propenoic acid	1.607	72	115.7	2.89
Glucose	0.5	180	90	2.25
CO_2	2.727	44	120	3
H_2O	197.2	18	3549.6	88.72
Total			4000.74	

The problem statement requires us to calculate of final broth in terms of mass percentages so we go back to building this table and we will down the amount which we have calculated ethanol has been calculated has 2.727 kilo moles propionic acid final broth is 1.07 kilo moles glucose in the final broth is 0.5 kilo moles and carbon dioxide is 2.727 kilo moles and water is 197.2 kilo moles.

The molecular weight for each of these are unknown and they are 46, 72, 180 44 and 18 using the molecular weight we can calculate the masses as the product of molecular weight and the number of moles to get the masses as 125.44 kilo grams 115.7 kilograms 90 kilograms, 120 kilograms and 3549.6 kilo grams. The summation here would come to 4000.74 kilograms one thing you would notice is we had 4000 kilo grams of feed present initially the value we are getting here is slightly off.

This is not because of mass being created this is just because of rounding of errors if we have not rounded of if we had used all the decimals we would get exactly 4000. So the numbers which we have used are slightly off because of rounding of errors so using this total mass and the individual masses for components we can calculate the mass percentages as 3.14, 2.89, 2.25 3 and 88.72.

So we have been as ked to calculate the mass percentages of ethanol and propionic acid in problem which comes out to be 3.14 and 2.89% which this we have come to the conclusion of this problem using extent of reaction method. As an exercise I would want you to perform the same calculation using molecular species balances and verify if you get the same answers with these three techniques namely the molecular species, balance atomic species balance and the extent of reaction technic.

You are now fully equipped to solve it any material balance problem containing wither single or multiple reaction. In the next class we will talk about reaction which happens in series thank you.