**Material and Energy Balances**
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**Module No # 03**
**Lecture No # 14**
**Material Balance Calculations for multiple Units Reaction – Part 1**

Hello everybody welcome to today's calculation on material balance calculation for system which have reactions and multiple units.

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Multiple units

- Most industry processes are multiple unit processes
- The reactants might need pre-processing
- The products need to be purified

Why multiple units? As I had mentioned already most industrial processes required multiple units you very rarely see a single unit process in industrial scale. So this means we also need to learn how to perform material balance calculation for multi-unit process. And in case of processes with reactions you usually have a reactor which is fed with the reactor.

In many cases these reactants might have to be preprocessed they might have to be mixed or they might have to be treated before we sent to the reactor and this could be a step or a unit ahead of the reactor. You could also have downstream operations down the reactor which could require the purification of the product any product you want to ultimately want sell in the market would have to meet certain standards.

So it might be because of purity it might be because of certain quality control there might be different reasons for making sure that the final product is of a certain grade and this can be accomplished only by separation processes which will follow the reactants. So as we mentioned earlier no reaction goes to completion in an industrial setup which means you will have a mixture of reactants and product which have been formed so to get a pure product which can be sold you have these downstream operations and that you might also want to recover the reactants and reuse the same.

The reactants are going to cost the money which means the industry would not want to throw them away. So recover these reactants is also a critical aspect for any process so for these reasons we always have downstream operations. So these separation processes would also have to be considered while you perform material balance calculations. Here will perform a few examples problems which take these things into account.

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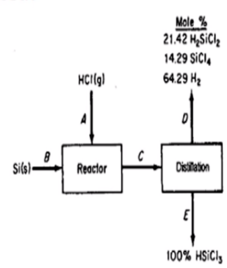
## Example #1

- Metallurgical-grade silicon is purified to electronic grade for use in semiconductor industry by chemically separating it from its impurities. The Si metal reacts in varying degrees with hydrogen chloride gas at 300°C to form several polychlorinated silanes. Trichlorosilane is liquid at room temperature and is easily separated by fractional distillation from the other gases. If 100 kg of silicon is reacted as shown in Figure, how much trichlorosilane is produced?




So here is the first example problem metallurgical grade silicon is purified to electronic grade for use in semiconductor by chemically separating it from is impurities the silicon metal reacts in varying degree with hydrogen chloride gas in 300 degree Celsius to form several polychlorinated silanes. Trichlorosilane is liquid at room temperature and is easily separated by fractional distillation from the other gases.

If 100 grams of silicon is reactant as shown in the figure how much trochlorosilane is produced? So the process is given as I had mentioned earlier here you have a reactor and a downstream which is a distillation column. So silicon which is coming into the reactor reacts with hydrogen chloride gas to form different silanes and trochlorosilane which becomes a liquid at room temperature is separated through the distillation process and the rest of the material leave as volatile gases.

So this is what would the system gives now let us see how we can go about solving this material balance problem.

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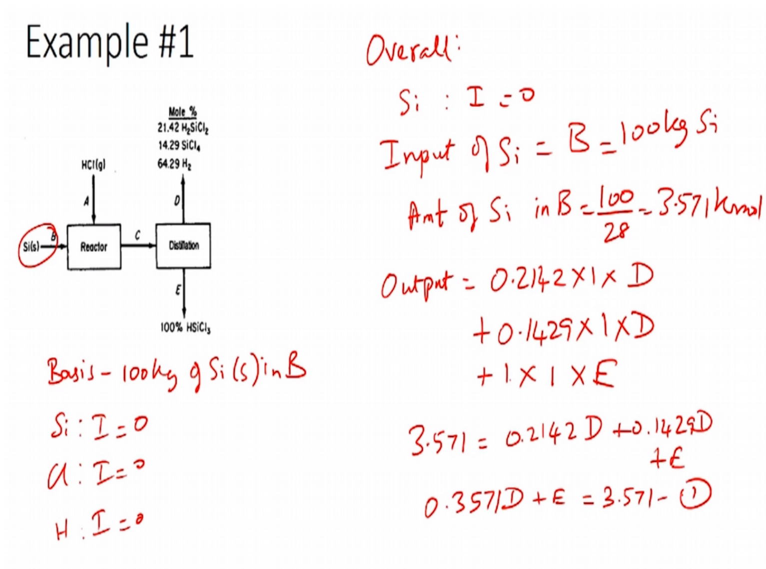


For any material balance problem the first step is to identify the basis the problem statement clearly gives 100 kilograms of silicon being treated so taking that into consideration you will take the basis as 100 kilograms of silicon fed to the reactor. So base is 100 kilograms of silicon solid in the feed which is B so which is this feed. Now we can write different equation so here we need to calculate the amount of trichlorosilane that is produced.

So for doing this we could either write component balances or we can write atomic balance so here I have chosen to write atomic balances instead of molecular species balances. So what atomic balances can we write so for this system we can write silicon balance chlorine balance and hydrogen balance. As we have mentioned earlier for atomic balances you do not have a generation or consumption term accumulation would be 0 at steady state so all these equations would implied to input = output so all these three is input = output only.

Now let us start writing the balance equation for silicon so silicon is entering as silicon solid through the feed B so here what is the system we want to choose. So unlike the previous problems we do not have only the reactor so we have a reactor and distillation column so we need to identify the system we would want to start with here we have the information regarding the feed which is entering into the reactor and we also have the information about the products leaving the distillation column.

However we do not have information about the stream which is connecting the reacting to the distillation column so this means taking the overall system would be the most appropriate way to approach the problem considering the overall system the silicon balance can be written as for the overall system silicon balance is input = output so input is input of silicon is only through the stream B which is 100 kilograms or silicon.

So the base is has been taken as 100 kilograms silicon based on the information given in the problem however if you see the composition of the stream which is leaving the reactant in the distillation column you find that the composition is given in terms of mole percentages it is a gas and conventionally the composition is given as mole percentages which is was it is been followed here also.

This means using masses for silicon would require the mole percentages to be given as mass percentages instead we can also convert the basis for silicon which is in 100 kilograms 2 moles so that we can use directly so for this reason we will convert the mass of silicon into moles which will give it has the amount silicon in the would be equal to 100 / 128 which is the molecular weight giving us 3.571 kilo moles.

So 3.571 kilo moles of silicon is being fed to the system so now for the output you have silicon leaving in the form of H2HICL to SICL 4 and HSICL3. So all of these molecules have one atom of silicon so taking the mole percentages and number of atoms of silicon per molecule we can write the output as 0.2142 times 1 times D which is the number of atoms which is leaving per molecule of H2SICL2 in the stream D + you have 0.1429 times 1 times D which is the number of atoms of silicon leaving per molecule of SICL4 in the stream D + 1 times E which is the number of atoms of silicon leaving through the trichrlosilane which is HICL3 leaving through the stream heat.

So substituting this back into the silicon balance we get 3.571 = 0.2142 D + 0.1429 D + E so the equation simplifies as 0.3571D + E = 3.571. So let us call these as equation 1 now we can write balance for chlorine.

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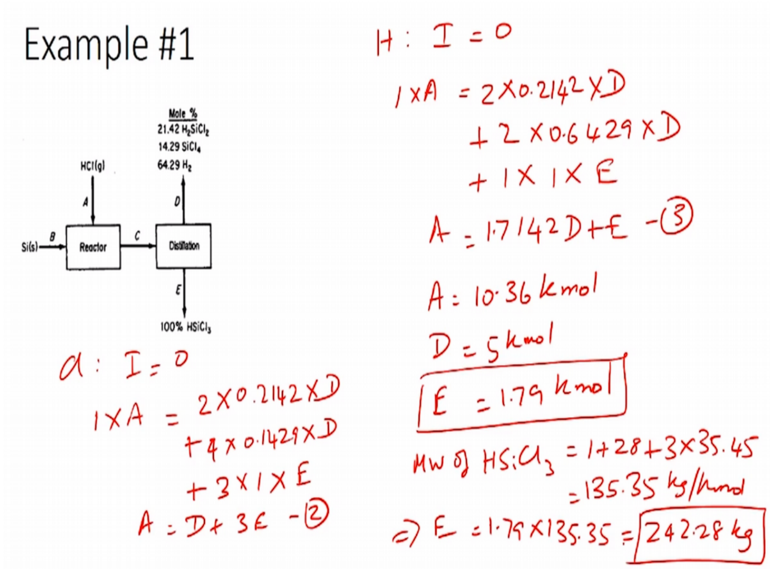


So the chlorine balance should be input = output again we have chlorine entering through the stream as entering through the system as HCL so you have one atom of chlorine per molecule of HCL. So taking that into consideration the input term becomes 1 times A and you have chlorine in the form of H2SICL2. SICL4 and HSICL3.

So you have two atoms of chlorine leaving H2SICL2 so that is two times 0.2142 times D + 4 times 0.1429 times D which is the number of atoms of chlorine leaving in the form of SICL4 you have 4 atoms of chlorine leaving per molecule of SICL4 through the stream D. And you also have 3 atoms of chlorine leaving through the stream 3 in the form of HSICL3 so we have three times 1 times E.

So this equation then can be simplified as A = B + 3E so let us call this equation number 2 so next we can write the balance equation for hydrogen. The hydrogen balance again which is input

= output using the same principles used till now input for hydrogen would 1 times A = 2 times 0.214 2 times D + 2 times 0.6429 times D and + 1 times E so this equation can be simplified as A= 1.71 42 D + E so this would be equation number 3.

Now we have 3 equations and 3 unknowns A, D and E solving for A, D and E using these three equations we get A = 10.36 kilo moles sorry B = 5 kilo moles and E = 1.79 kilo moles. So we have been asked to calculate the amount of trichlorosilane which is produced so that would being E. So we get 1.79 kilo moles. So we have been asked to calculate the amount of trochlorosilane which is produced so that would be stream E so we get 1.79 kilo moles of trichlorosilane being produced per 100 kilo grams of silicon which is fed.

Converting this to mass we will just have to multiply this with the molecular weight so molecular of trichlorosilane would be HISICL3 is 1+ 28 + 3 times 35.45 giving you a value of 135.35 kilograms per kilo moles. So this means E = 1.79 times 135.35 equal to 242.28 kilograms so for every 100 grams of silicon which is supplied you end up producing 242.28 kilograms of silicone. With this we end up calculated what has been asked for in the problem now let us move on to the next problem.

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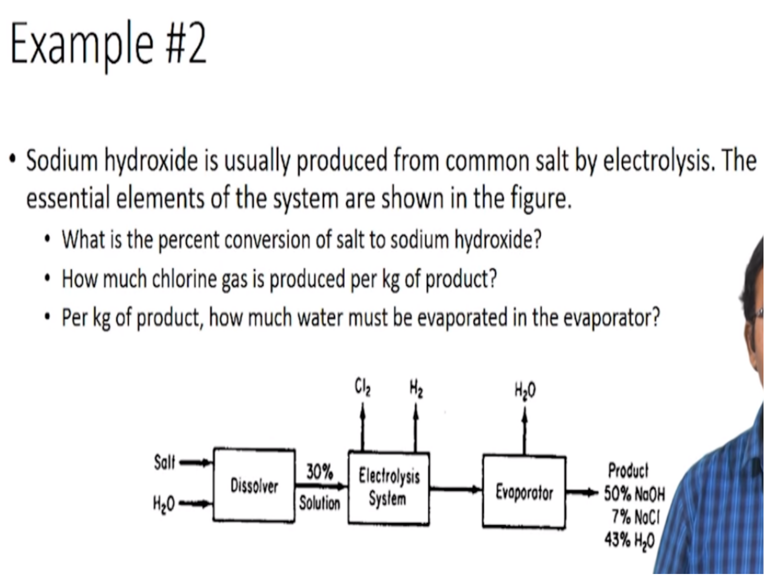


Sodium hydroxide is usually produced from common salt by electrolysis system. The essential elements of the system are shown in the figure what is the present conversion of salt to sodium hydroxide how much chlorine gas is produced per kilogram of product and per kilogram of product how much water much be evaporated by the evaporator. So if you look at the flow chart what you see is you have electrolysis system which is the reactor in our case.

So this salt solution which is fed to the electrolysis system is reacted to form sodium hydroxide and chlorine and hydrogen so you have salt solution which is prepared using a dissolver before the salt solution is fed to the electrolysis system the salt and water are mixed in a dissolver to product 30% salt solution which then enters into the electrolysis chamber and gets electrolyzed to product sodium hydroxide.

Then the sodium hydroxide solution you end up with is sent to an evaporator to get a desired composition which is given as 50% sodium hydroxide 7% NACL and 43% water as the product. So now that we have the system let us look at how we solve this problem.

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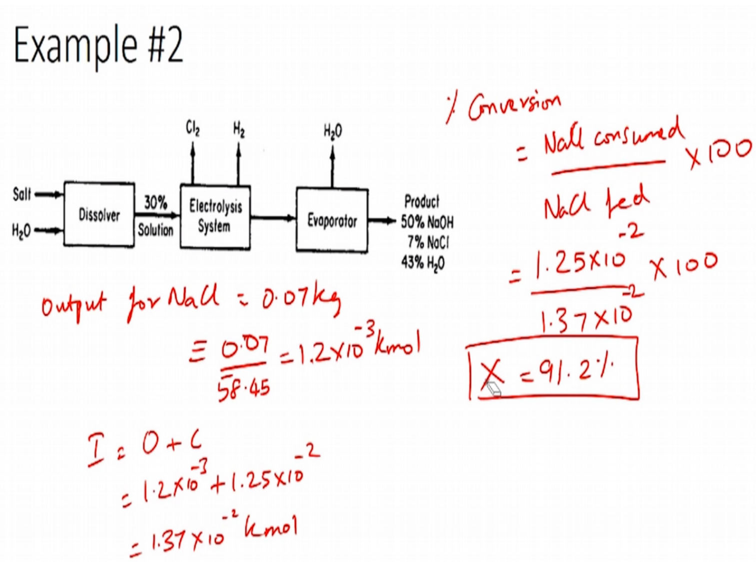


First think we need to identify here is although the process and the system as been given the chemical reaction itself has not been given to us however we have given what the reactors are and what the product are through the flow chart that has been provided to us. So you have salt and water entering into the system which means those two are the reactants and you have chlorine, hydrogen and sodium per oxide leaving as products in addition to unreacted water and NACL.

Taking these into consideration let us build the chemical reaction which would happen inside the electrolysis system so you have NACL reacting water to form NAOH + chlorine + hydrogen now that you have the equation you need to verify if it is balanced what you would see is it is not hydrogen and oxygen are not balanced so how do we go about this to make sure that hydrogen is balances we can have 2 here and here.

Thereby you have 4 atoms of hydrogen entering and 4 atoms of hydrogen leaving through the reactant product stream. So now you have two oxygen and 2 atoms of oxygen however sodium is not balanced here so you added 2 here thereby you ensure that sodium chlorine are also balanced. So 2 atoms of NA here and you have 2 atoms of chlorine entering here 2 atoms of chlorine leaving here you have 4 atoms of hydrogen entering and 2 + 2 atoms of hydrogen which is 4 atoms of hydrogen leaving 2 atoms of oxygen entering and 2 atoms of oxygen leaving.

So this is the balanced equation which we need to performing the material balance calculation so the next step is to identify the basis for the problem. So the problem repeatedly asked for different information based on 1 kilograms of product being so taking that into consideration you will assume that basis to be 1 kilogram of product stream which is being formed so the basis for the system would be 1 kilogram of product.

So this means you have 0.5 kilogram NAOH 0.07 kilogram of NACL and 0.43 kilograms of H2O in the product stream. So now the first question is to identify the conversion of NACL for this we need to know how much of NACL is entering the system we already know the amount of NACL is leaving the system if we know how much NACL is consumed then we can calculated conversion the amount of NACL consumed can be obtained by knowing the amount of NACL entering and amount of NACL leaving.

So for this reason we will start with NACL balance so NACL balance would be input – output + generation – consumption = accumulation at steady state you do not have accumulation NACL is the reactant is not being produced so there is no generation so you end with input = output + consumption so we need to calculate consumption so consumption = input – output. So now how do we go about a consumption and input term.

So the consumption term would be equal to the generation of NAOH so that is what stoichiometric says based on the reaction2 moles of NACL consumed will result in formation of 2 moles of NAOH. You know that 0.5 kilograms of NAOH is produced in the final product so this means we can calculate the consumption of NACL using the number of moles of NAOH produced.

Consumption of NACL is therefore equal to generation of NAOH so generation of NAOH = 0.5 kilograms which is equivalent to 0.5 divided by 40 which is 1.25 times 10 power -2 kilo moles of NAOH. So therefore consumption of NACL would also be equal to 1.25 times 10 power -2 kilo mole. Now that we have the consumption term we can calculate the input term as soon as we identify the output.

We already know that the output for NACL 0.7 kilograms so this is equivalent of 0.07 divided by 58.45 which is molecular weight NACL giving you 1.2 times 10 power -3 kilo moles of NALC which is leaving the system. So your input = output + consumption which is 1.2 times 1 power – 3 + 1.25 times 10 power -2 giving you 1.37 times 10 power -2 kilo moles being fed. So now we have the input and the output terms and consumption term for NACL.

If you recollect the definition of conversion it is the amount of the reactant consumed by the number of reactant fed. So based on that conversion would be NACL consumed divided by NACL fed. So here we have been asked for percentage conversion which means this multiplied by 100 so we know that NACL consumed is 1.25 times 10 power -2 and NACL fed is 1.37 times 10 power – 2 and 100

Giving us the percentage conversion as 91.2% so with this we have calculated the percentage conversion of NACL in this system. The next part of the problem ask us to calculate how much chlorine gas is produced per kilogram of product.

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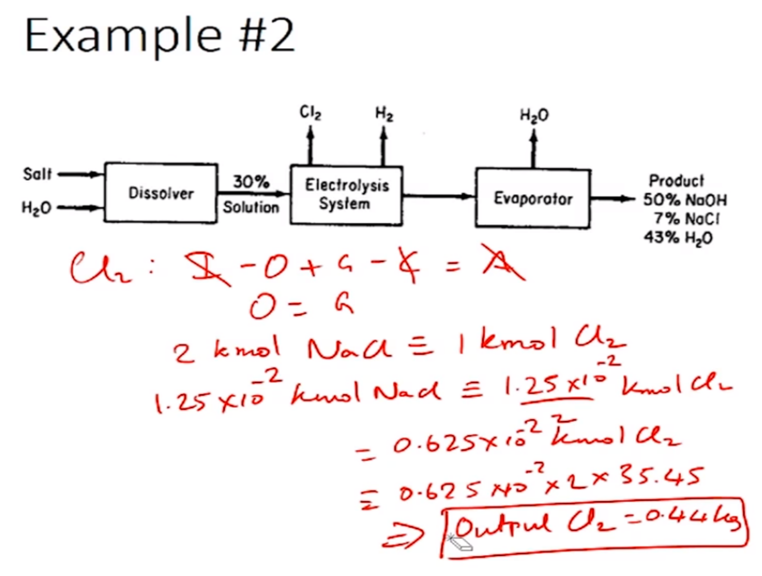


So we need to identify the amount of chlorine which is leaving through electrolysis system if we have go back to the balance equation chlorine would look like chlorine balance would look like input – output + generation- consumption = accumulation no accumulation at steady state chlorine is a product and it is no consumed you do not have any input for chlorine so thereby output = generation all we need to do is identify the generation of chlorine.

So if we look at the stoichiometry what we identify is for every two moles of NACL consumed you have 2 mole of being produced so you have 2 kilo moles of NAOH sorry NACL produced 1 kilo mole of chlorine being produce this would mean 1.25 times 10 power -2 kilo moles of NACL consumed would result in the formation of 1.25 times N power -2 divided by 2 kilo moles of chlorine which is 0.625 times 10 power -2 kilo moles of chlorine.

And if were to convert this to mass you will have to multiply this to molecular weight for chlorine and that would give us 0.625 times 10 power -2 times 2 times 35.45 giving us the final value of output for chlorine would be 0.44 kilo grams so with this we have calculated the amount of chlorine which is produced in the system per kilogram of product being formed.

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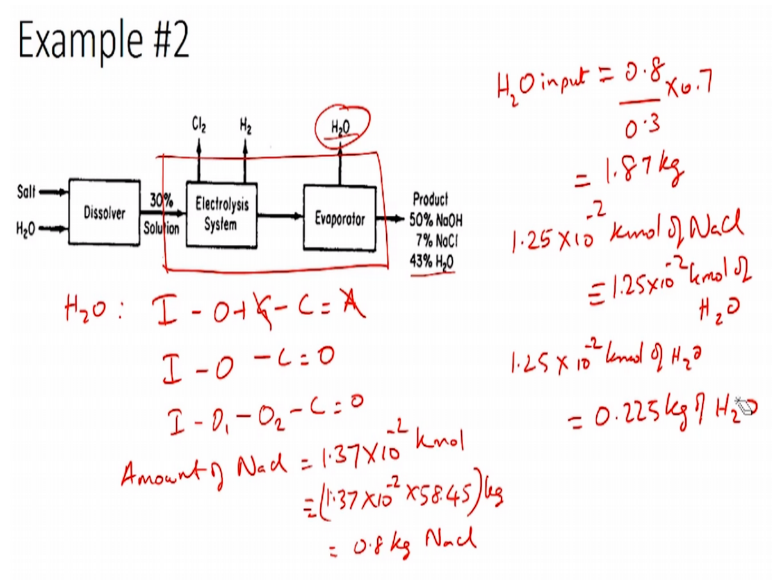


To calculate the amount of water leaving the evaporator as water vapor we need to perform a water balance we also need to identify what would be the ideal system to vapor so until now we have been using the overall system to perform the balances it did not matter that we did not have information of the amount of water entering because we were writing the balance for NACL and chlorine all the information we needed from the stoichiometric and the information about the product stream.

However to know how much water is actually entering the dissolver we do not have any information but we do have the information about the composition of the salt solution entering into the electrolysis system which means we need to now identify the new system to perform our balance equation.

Instead of considering the overall system we can write the balance equation for the electrolytic system + the evaporator so for this particular system we have chosen we have information about the input stream which gives us information of composition of NACL and water and we have information about the product stream which again have this information about the composition of water present in the product and in addition we have a product stream which is water vapor which is leaving the evaporator.

So we need to calculate this particular value now let us start writing the water balance for this particular system. The water balance would be input - output + generation – consumption =

accumulation at steady state water is not being generated as it is a reactant is only being consumed so you are left with input – output – consumption = 0. So this output terms as two different output you have one in the form of water leaving through the product and the other which is the water vapor leaving the evaporator.

So we will convert this into input – output 1 – output 2 – consumptions = 0 now we need to know how much of water is entering into the system what information do we have know the amount of NACL which is entering the system we already did this calculation and amount of NACL entering the system is 1.37 times 10 power -2 kilo moles so this would be 1.37 times 10 power -2 times 58.45 kilo grams which is 0.8 kilograms of NACL.

We know that the stream which is entering into the electrolysis system is 30% NACL so which means the remaining 70% would be water so H2O input to the system water input to the system would be equal to 0.8 divided by 0.3 times 0.7 which is 1.87 kilograms. So with these we can calculate the amount of water entering into the system we now need to identify how much water has been consumed by the reaction.

If you look at the reaction stoichiometric you would identify that for every mole of NACL reactor one mole of water also reactor it is given as two moles of NACL + two moles of water reacting so we based on that we can identify that for 1.25 times 10 power -2 kilo moles of NACL reactant would mean that 1.25 times 10 power -2 kilo moles of water also consumed. So this would mean that 1.25 times 10 power -2 kilo moles of water which weights 0.225 kilograms of water has been consumed.

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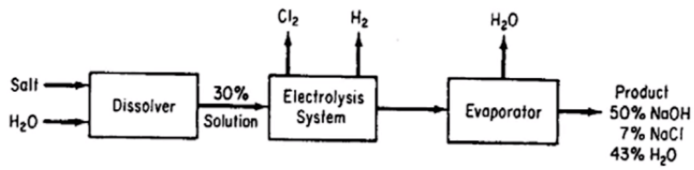
# Example #2




$$O_2 = 0.43\ kg$$

$$I - O_1 - O_2 - C = 0$$

$$(Output)_{H_2O(v)} = 1.87 - 0.43 - 0.225$$

$$\boxed{H_2O(v) = 1.215\ kg}$$

So we now have information about the water which is entering and the water which is consumed we need to identify how much water is leaving the system so the water which is leaving the system in the form of the product is O2 which is 0.43 kilograms so based on this we have all the information we have input we have output 2 and we have consumption.

We just need to calculate output1 which is the water leaving in the form of the water vapor would be input which is 1.87 – output in the product stream which is 0.43 – consumption which is 0.225 giving you the total amount of water evaporated as 1.215 kilograms as the water leaving the evaporator in the form of water vapor.

With this we have solved this problem and identified all the basic information has been asked for. In the next class we will look at relatively more complicated problem with multiple processes and multiple units and we will try to read the problem statement and draw of the flowchart which would be then used for performing the calculation thank you.