**Plant Design and Economics**
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**Lecture - 04**
**Flow Diagrams - Mass and Energy Balance**

Welcome to lecture 4 of Plant Design and Economics. In our previous lecture, we have talked about process flow diagrams. Now we have seen that process flow diagrams contains mass balance informations, energy balance informations for all major steps. So in this lecture we will talk about mass and energy balance in some detail.

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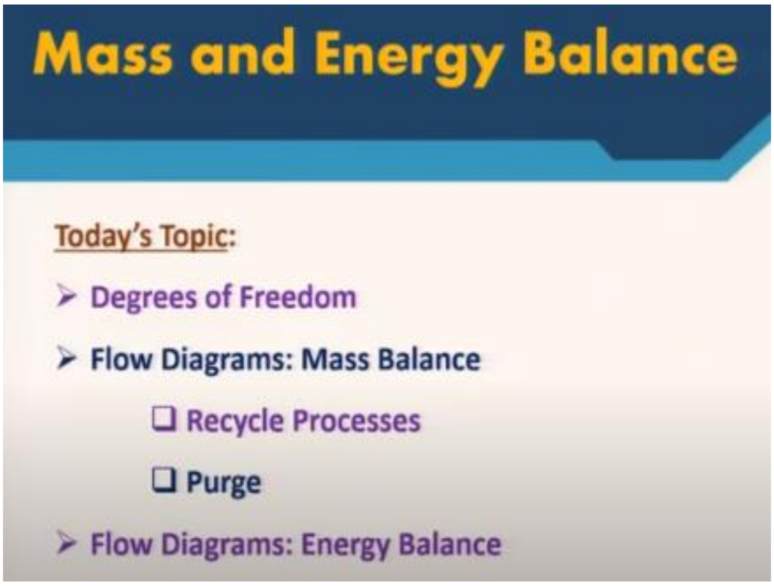


So this will be today's topic. We will define degrees of freedom. We will talk about mass balance in flow diagrams with recycle with purge and also we will briefly talk about energy balance.

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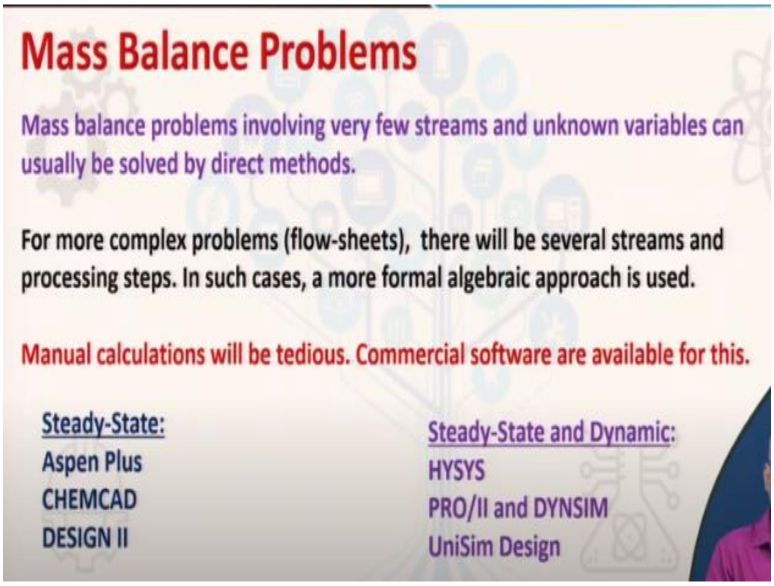


Now mass balance problems involving very few streams and unknown variables can easily be solved by direct methods. But for complex problems meaning if you have a complex flow sheet there will be several streams and processing steps. In such cases, a more formal algebraic approach is used. Manual calculations will be tedious and commercial software are available for this.

Some of the softwares that are available are given here. Aspen Plus, CHEMCAD, DESIGN II. They will perform steady state simulations. Then there are softwares which will perform both steady state and dynamic simulations, HYSYS, PRO/II and DYNSIM, UniSim Design. All these softwares will be extremely useful as they perform both steady state simulations and dynamic simulations and performing mass balance, energy balance will all be very easy.

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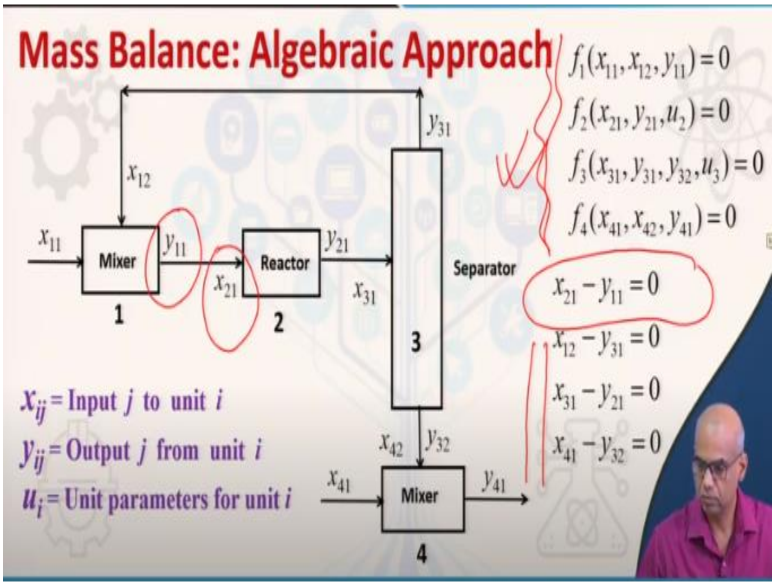


Now what you see is a block diagram for a simple process. So there are four equipment or four units. 1 is mixer, 2 is reactor, 3 is separator and 4 again another mixture. So first x 11 input goes to mixer. Then the output of the mixer goes to reactor. Output of the reactor goes to separator. So from separator one stream goes as recycle stream to mixer 1 and the other stream from the separator goes to mixer where it mixes with another stream x 41 and you get output as y 41.

Now let us use this nomenclature. x ij represent input j to unit i. So x 11 is input 1 to unit 1. x 31 will be unit 1 input 1 to unit 3. Similarly, x 12 will be input 2 to unit 1. Note that there is one input here, there is another input here. Similarly, y ij represent output j from unit 1. So y 11 will be output 1 from unit 1. y 31 will be output 1 from unit 3. y 32 will be output 2 from unit 3.

Now once we understand this nomenclature, let us try to understand that around each unit around each unit you can write mass balance or energy balances which will be expressed as a mathematical function of these inputs and outputs and also other unit parameter that may be associated with the units. For example, say reactor separator may have certain unit parameters associated with these units.

So the mass balance equation or energy balance equation can be written around each unit and they will be functions of these inputs, outputs and unit parameters. Now if these functional forms or if these equations are simultaneously solved we will get the mass balance and the energy balance associated with each stream. Now note that every unit has been associated with input and output.

So y 11 is the output 1 from unit 1. x 21 is the input 1 to unit 2. But as the figure suggests, y 11 must be equal to x 21. So along with these equations, you must also have to solve equations like y 11 equal to x 21. In other words, x 21 – y 11 = 0. Similarly, all these equations needs to be solved simultaneously with these equations f 1, f 2, f 3, f 4 which represent mathematically energy balance or mass balance around each unit. These informations can be easily coded and can be solved on computers.

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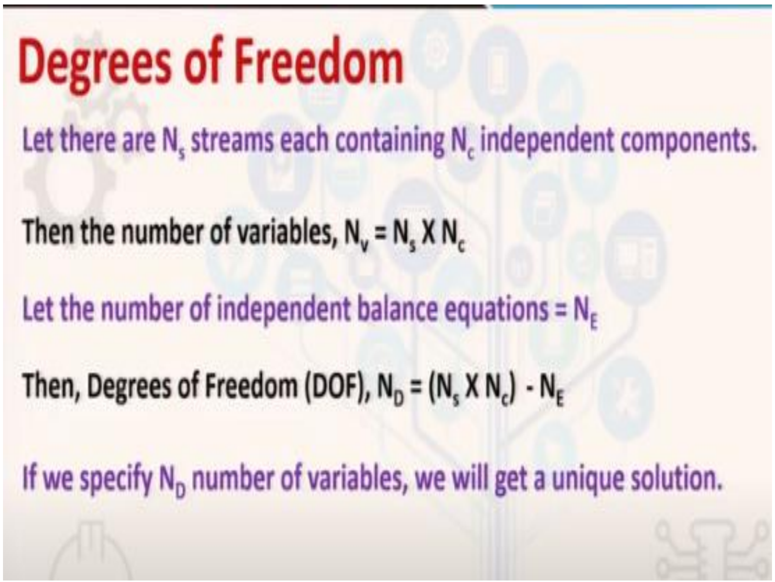


Now you know that degrees of freedom is defined as total number of variables minus number of independent equations. So let there be N s number of streams and each stream is associated with N c number of independent components. So each stream has N c number of components. So N s streams will have N s into N c number of variables. Let the number of independent balance equations be N E.

So degree of freedom is defined as N s times N c minus N E. So if we specify N D number of variables then your system will be uniquely defined, you get a unique solution.

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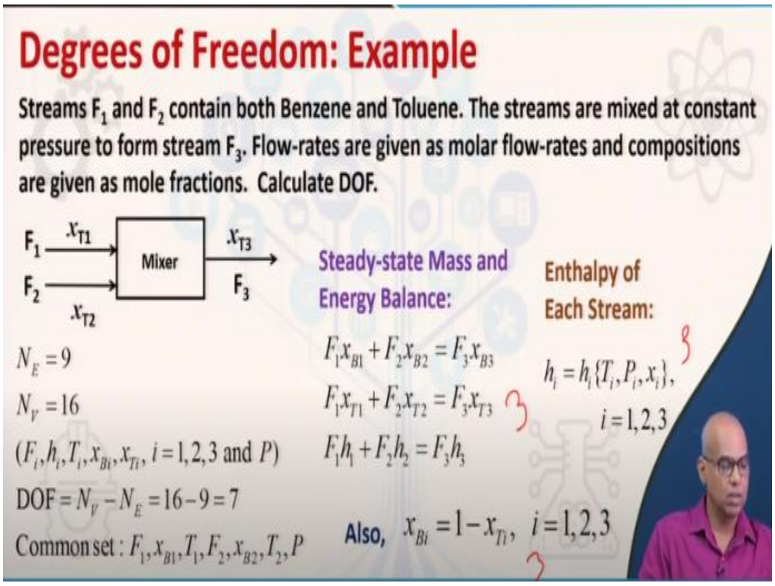


Now let us take an example for degree of freedom computation. The blog represents a mixer where stream F 1 and F 2 enters and stream F 3 comes out. Each stream F 1 and F 2 contain benzene and toluene. So the streams are mixed at constant pressure. Let the flow rates be molar flow rates and the compositions be mole fractions. So what balance equations can you write? We can write steady state mass and energy balance equations.

So x T1 is the mole fraction of the toluene, x B1 with the mole fraction of benzene. Similarly, for x B2, x B3. So you can write the first balance equation as moles of benzene that enters and moles of benzene that comes out. Similarly an equation on toluene you can also write energy balance equation. Enthalpy that goes in with F 1 plus enthalpy that goes in with F 2 will be equal to enthalpy that comes out with F 3.

So these are three mass balance and energy balance equations. Now you can also write relation for enthalpy of each stream. So you can write three relations representing enthalpy for stream 1, stream 2 and stream 3. So h 1, h 2, h 3 all are functions of temperature of the stream, pressure of the stream and composition of the stream. We also have the relation that sum of the mole fractions equal to 1.

So x B1 = 1 - x T1. x B2 = 1 – x T2. x B3 = 1 – x T3. So how many equations we have? We have 9 equations, 3 here, 3 here and 3 here. How many variables are here? We have flow rate, enthalpy, temperature, benzene mole fraction and toluene mole fraction. These 5 quantities for each stream. So 5 into 3 15 plus we have pressure so 16. So we have 16 number of variables.

So degrees of freedom will be computed as 16 – 9 = 7. So if you want to completely define your system, if you want to get unique solution, you have to specify 7 variables. The common sets are the flow rate, mole fraction of benzene and the temperature for stream 1. The same maybe for steam 2, so 6. And then pressure 7. So these are the 7 common sets which will be chosen to completely specify the system.

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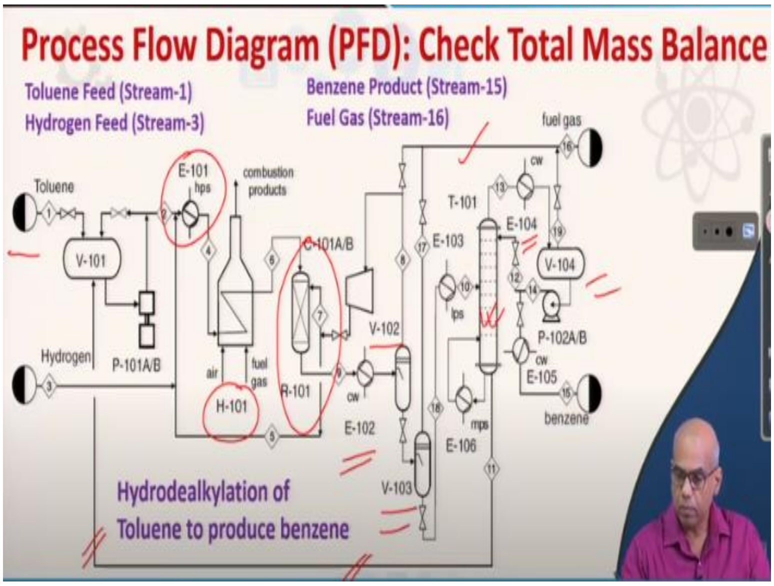


Now we are familiar with this flow sheet. This is hydrodealkylation of toluene to produce benzene. So the overall reaction is toluene plus hydrogen equal to methane plus benzene. So fresh toluene is mixed with recycled toluene. Then it is pressurized and mixed with hydrogen. Then the mixture is first heated with the heater E-101. And then again with the furnace H-101 to raise the temperature.

The temperature is raised to around 600 degrees Celsius. Then the stream goes to the reactor, R-101 which is a packed bed reactor, is a catalytic reactor in which the reaction takes place. The effluent from the reactor is cooled with E-101. And then the cold stream is phase separated using phase separators V-102 and V-103. First the gas stream is separated.

So whatever hydrogen that is possible to recover is recycled back to the reactor. Look at the stream number 7 and the other stream which is predominantly methane is taken out as fuel gas. Now the liquid stream for V-103 is sent to the distillation column where the liquid mixture is separated. The lighter component is benzene is taken from the top of the distillation column, cooled using E-104 and then stored.

The heavier component is toluene taken from the bottom of the distillation column and recycled. So this is how the hydrodealkylation of toluene to produce benzene takes place. Now we want to see whether the total balance is maintained or not. We know that stream table will be there which will give me the detailed information about each stream.

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**Process Flow Diagram (PFD): Stream Table**

| Stream Number | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|---|---|---|---|---|---|---|---|---|
| Temperature (°C) | 25 | 59 | 25 | 225 | 41 | 600 | 41 | 38 |
| Pressure (bar) | 1.90 | 25.8 | 25.5 | 25.2 | 25.5 | 25.0 | 25.5 | 23.9 |
| Vapor Fraction | 0.0 | 0.0 | 1.00 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 |
| Mass Flow (tonne/h) | 10.0 | 13.3 | 0.82 | 20.5 | 6.41 | 20.5 | 0.36 | 9.2 |
| Mole Flow (kmol/h) | 108.7 | 144.2 | 301.0 | 1204.4 | 758.8 | 1204.4 | 42.6 | 1100.8 |
| Component Mole Flow (kmol/h) | | | | | | | | |
| Hydrogen | 0.0 | 0.0 | 286.0 | 735.4 | 449.4 | 735.4 | 25.2 | 651.9 |
| Methane | 0.0 | 0.0 | 15.0 | 317.3 | 302.2 | 317.3 | 16.95 | 438.3 |
| Benzene | 0.0 | 1.0 | 0.0 | 7.6 | 6.6 | 7.6 | 0.37 | 9.55 |
| Toluene | 108.7 | 143.2 | 0.0 | 144.0 | 0.7 | 144.0 | 0.04 | 1.05 |

So here it is. So stream numbers are given. This is the part of the stream table and all the informations temperature, pressure, vapor fraction, mass flow rate etc., are all available. Now to check the total mass balance, we have to look at how much of toluene and hydrogen enters and how much of fuel gas and benzene comes out. So we have to focus our attention on stream number 1 and 3 as input and stream number 15 and 16 as output.

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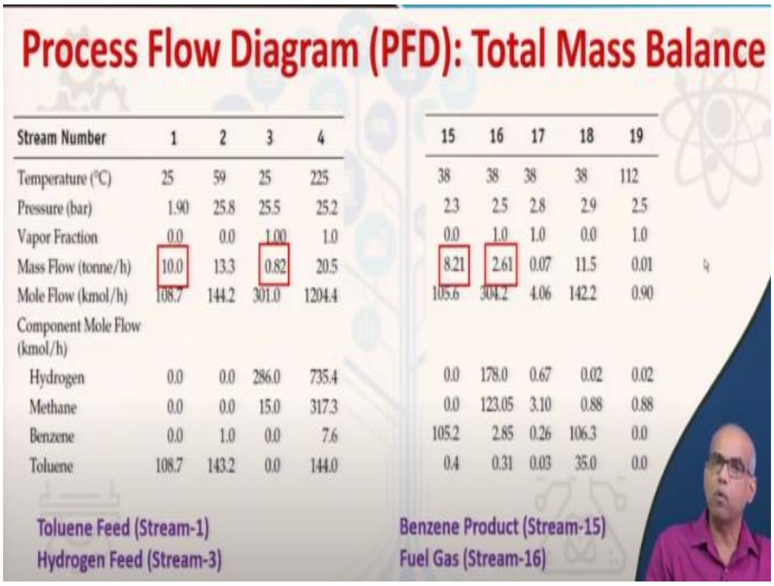


So let us look at the stream table. So what goes in is 100 + 0.82 tonnes per hour which is 10.82. What comes out is 8.21 + 2.61. So that is also 10.82 tonnes per hour.

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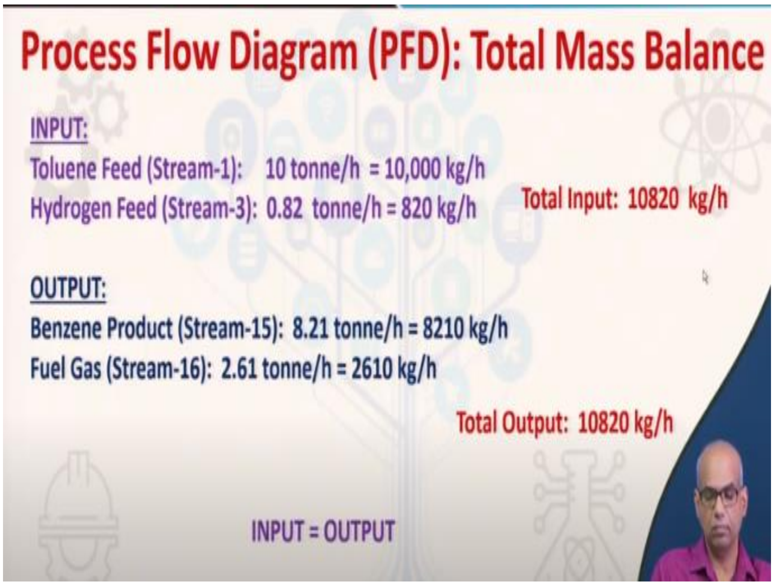


So mass balance is maintained, input equal to output.

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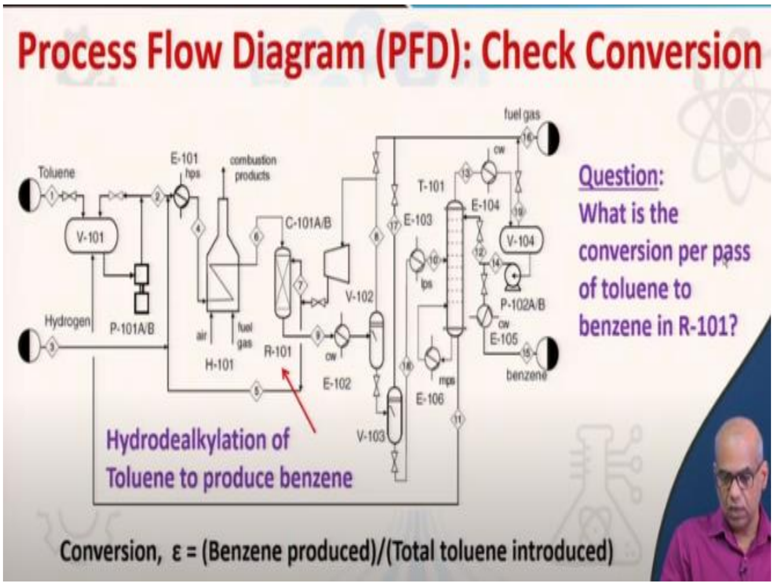


Next we let us take the conversion per pass of toluene in R-101. So you ask the question what is the conversion per pass of toluene to benzene in the reactor R-101. Let us define the conversion as benzene produced divided by total toluene introduced.

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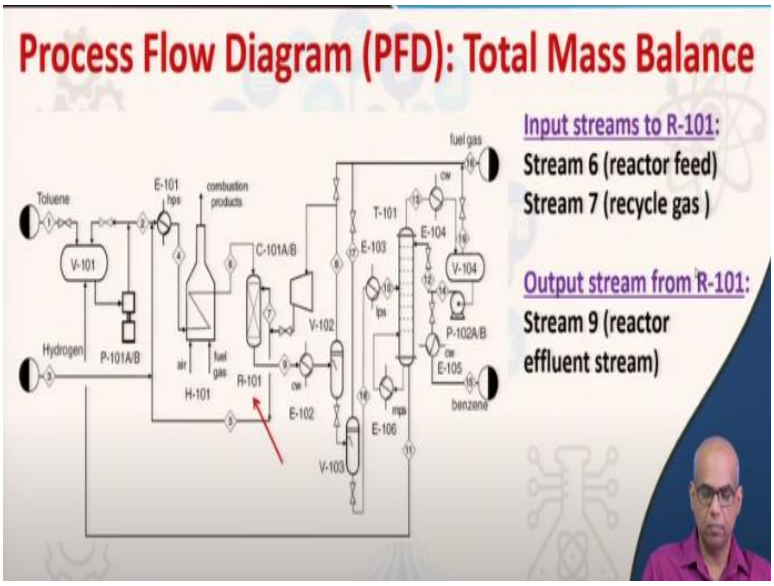


So let us look at the input streams to the reactor and the output streams from the reactor. Streams number 6 and 7 are the inputs. Stream number 9 is the output stream from the reactor.

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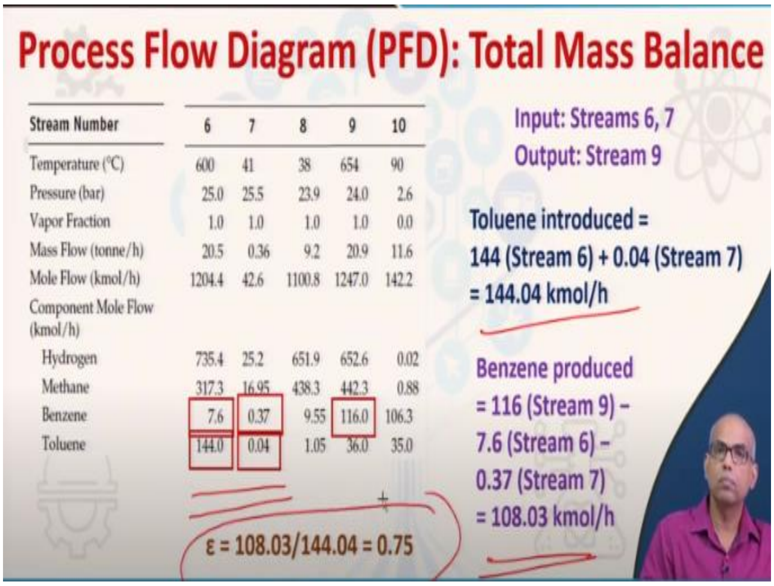


So now, look at the stream table corresponding to this stream. So find out the total toluene that is introduced which is introduced with stream number 6 and stream number 7. The quantity is 144.04 kilo mole per hour. Similarly, compute the benzene produced which will be benzene that goes with stream number 9 minus concentrated benzene in stream number 6, benzene in stream number 7.

So that will give you 108.3 kilo mole per hour. So thus their ratio will give you the conversion. So this way you can compute the conversion.

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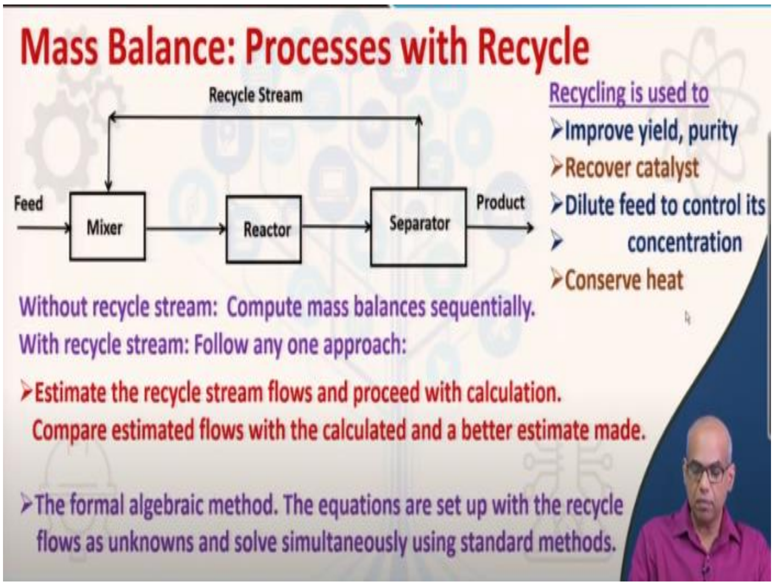


Now let us consider process with recycle. Recycling is frequently used in chemical process industry. So look at the schematic. A stream from the separator is fed back to the mixer. So feed goes to mixer from where it goes to reactor. The effluent goes to separator. From the separator product stream is taken out but unreacted stream maybe send back and mixed with the raw feed.

And this will be again fed to the reactor. This will improve yield. This will improve purity. You may use recycle to recover catalyst. You may want to dilute feed to control its concentration. You may also conserve heat. So the recycling will serve several purpose. Without recycle stream, we can compute mass balance sequentially. There would not be any problem.

With recycle stream you cannot compute mass balance in a straightforward sequential manner. We have to do any of the following. Estimate the recycle stream flows and proceed with calculation. Compare estimated flows with the calculated and a better estimate is then made. Other approach will be you adopt a formal algebraic method.

The equations are set up with the recycle flows as unknown and solved simultaneously using standard methods.

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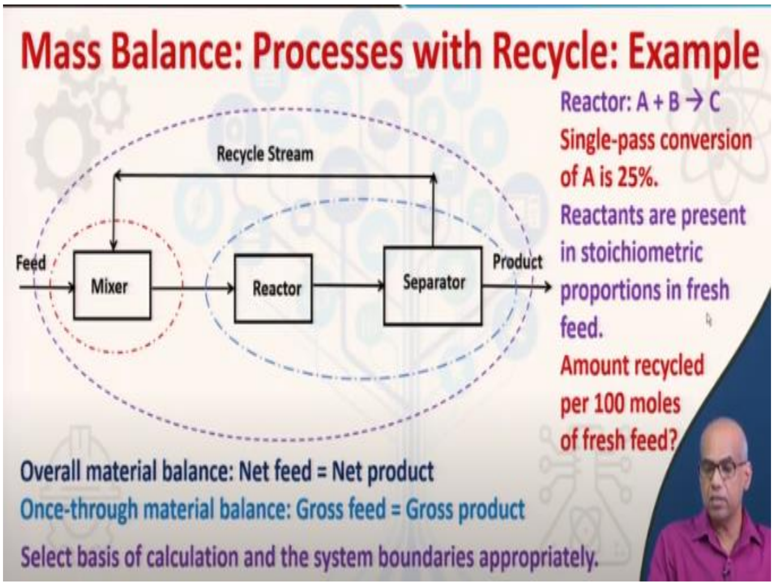


Look that you can draw several system boundaries and you have to select basis of calculations and system boundary appropriately. In the schematic, we have drawn three system boundaries. One around only mixer, one around reactor and separator and another one which encompasses the entire schematic of the plan. You can write two types of balances.

Overall material balance, where you equate net feed with net product. You can also write once-through material balance, where we will equate gross feed with gross product. Now let us ask this question. In the reactor a reaction takes place which is A plus B goes to C. Single-pass conversion of A is 25%. Let us assume that reactants are present in stoichiometric proportions in fresh feed. What should be the amount recycled per 100 moles of fresh feed?

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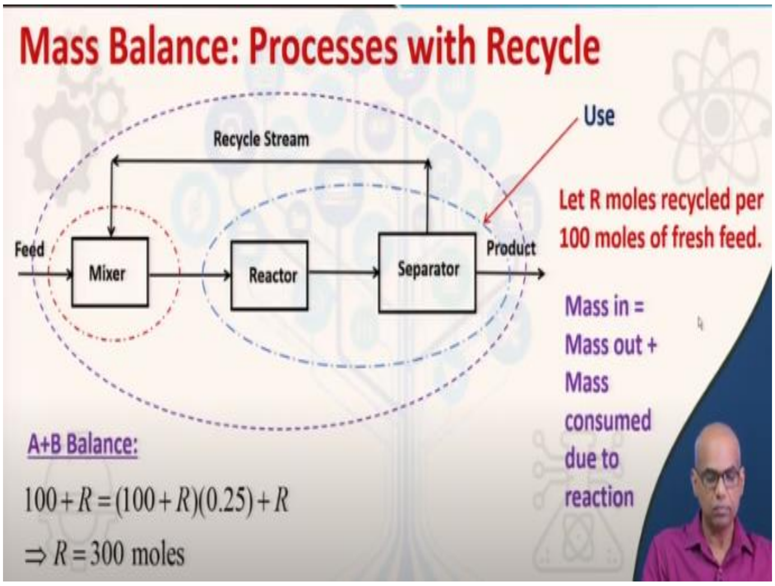


So which system boundary to choose? Let us choose the system boundary around reactor and separator. L R moles recycle per 100 moles of fresh feed. Now you write the mass balance as mass in will be equal to mass out plus mass consumed due to reaction. So now write A + B balance. What is mass in? 100 + R with recycled stream.

Then what goes out is 100 + R 25% of it plus R. This gives you R = 300 moles. So 300 moles must be recycled per 100 moles of fresh feed.

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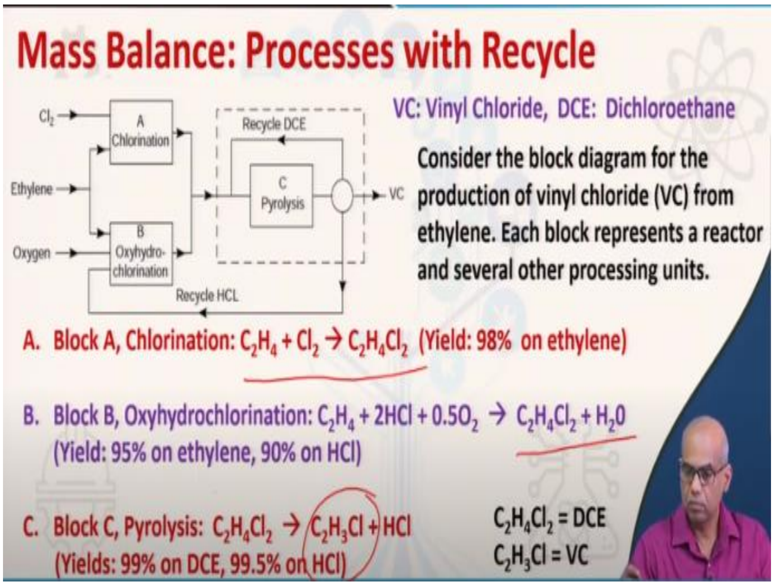


Now let us take a little bit more complicated process with recycle. Consider the block diagram for the production of vinyl chloride from ethylene. There are 3 blocks here. Each block represents a reactor and several other processing units. So you have 3 blocks A, B, and C. In the block A chlorination takes place. In block B, oxyhydrochlorination takes place. And in block C pyrolysis take place.

So in block A the chlorination takes place and the yield is 98% on ethylene. Here in block A ethylene and chlorine produces dichloroethane. In block B oxyhydrochlorination takes place and it also produces dichloroethane. In the block C, there is pyrolysis of dichloroethane and vinyl chloride is produced along with HCl.

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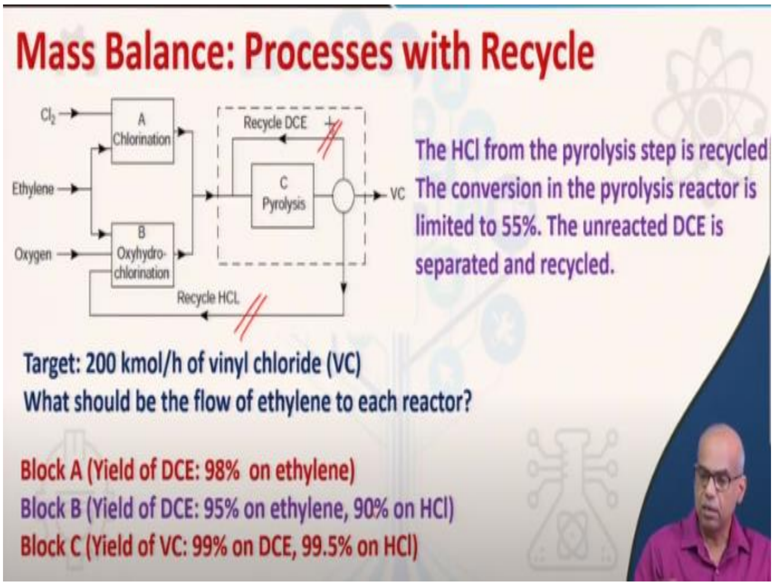

Now if you target 200 kilo mole per hour of vinyl chloride, what should be the flow of ethylene to each reactor? That is the question. Not here the HCl from the pyrolysis step is recycled. The conversion in the pyrolysis reactor is limited to 55%. And the unreacted dichloroethane is separated and recycled. So HCL is recycled, dichloroethane which is unreacted is separated and recycled.

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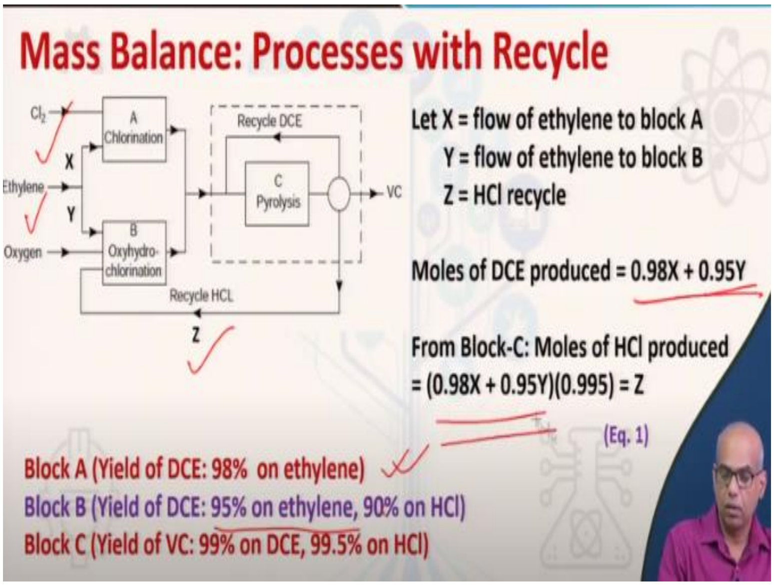


Now let us assume that X be the flow of ethylene to block A and Y be the flow of ethylene to block B and Z equal to HCl recycle. What is the moles of dichloroethane that is produced? Note the yield of dichloroethane is 98% on ethylene and in block A. So you get 0.98X. X is the flow of ethylene to block A. So you get 0.98X dichloroethane.

Similarly you get 0.95Y dichloroethane because Y goes to block B where the yield is 95% on ethylene. So the moles of dichloroethane produced is 0.98X + 0.95Y. From block C where pyrolysis takes place you can find out that moles of HCl produced will be 99.5% of this quantity. So this gives me one equation.

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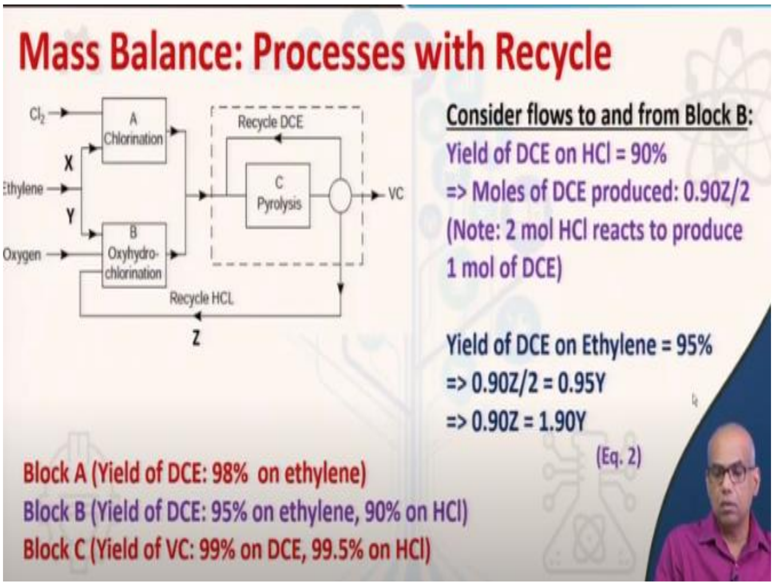


Next, let us consider flows to and from block B. Yield of dichloroethane on HCL is given as 90%. So moles of dichloroethane produced will be 0.90Z by 2 because 2 moles of HCL reacts to produce 1 mole of dichloroethane. Again, yield of dichloroethane on ethylene is 95% in block B. So that gives me 0.95Y moles of dichloroethane in block B.

So 0.90Z by 2 must be equal to 0.95Y. So this gives me another equation, which I call equation 2.

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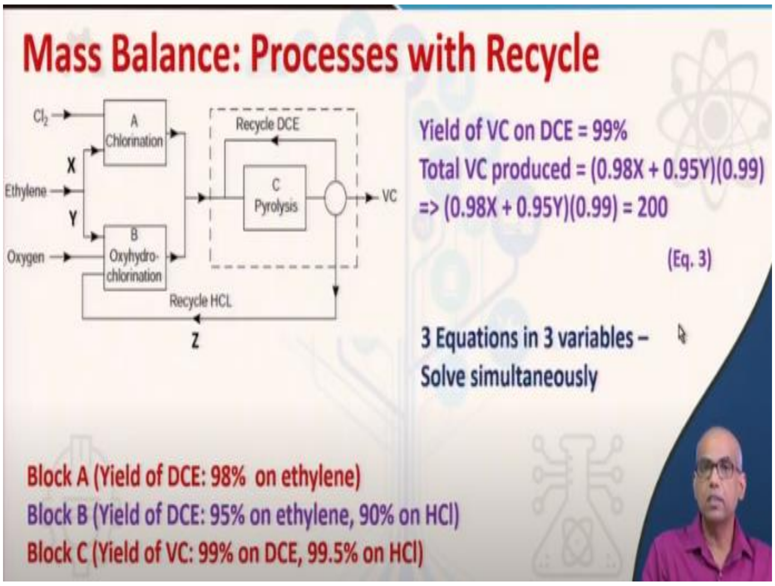


Finally yield of vinyl chloride on dichloroethane is 99%. So total vinyl chloride produced will be the total moles of dichloroethane which is 0.98X + 0.95Y multiplied by 0.99. This must be equal to my target 200. So this gives me third equation. So now, we have three equations and three variables X, Y, Z. It is easy to solve. We can solve simultaneously.

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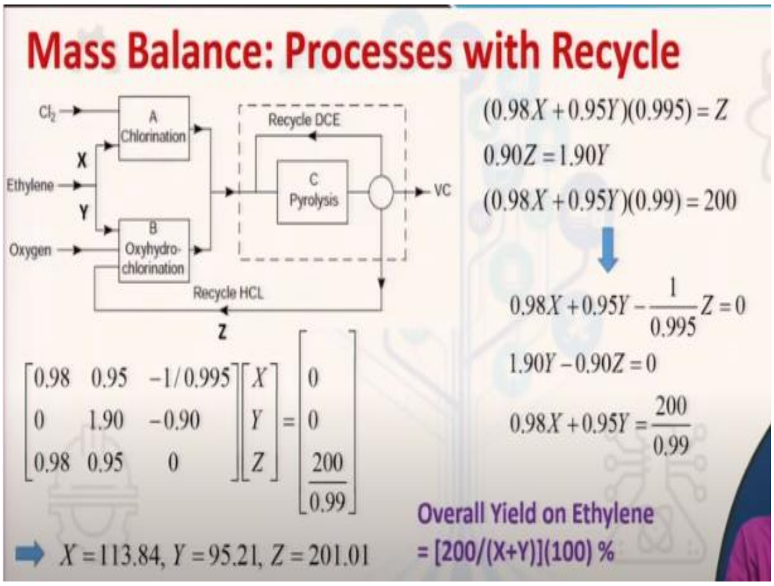


We can write this equation in standard matrix form like Ax equal to B and you can also solve as A inverse B, which gives you X = 113.84, Y = 95.21, and Z = 201.01. So the flows of ethylene to block A is 113.84 and to Block B is 95.21, recycle is 201.01. You can also solve these three equations by substitution method also.

Now once you have got these values you can find overall yield on ethylene as my target vinyl chloride 200 divided by total moles of ethylene that is X + Y. So we can express it as percentage.

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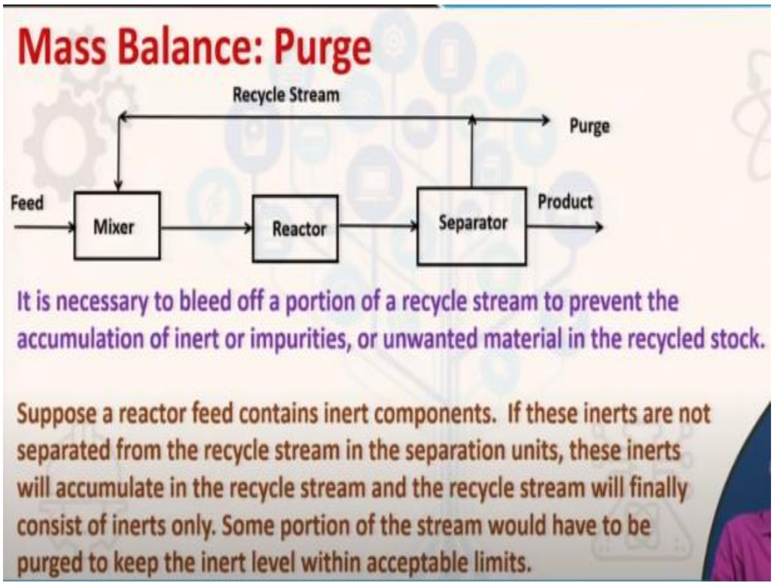

Now let us look at purge. It is necessary to bleed off a portion of a recycle stream to prevent the accumulation of inert impurities or unwanted material in the recycle stock. Suppose, the reactor feed contains inert components. If these inerts are not separated from the recycle stream in the separation units, these inerts will accumulate in the recycle stream and the recycle stream will finally consist of inerts only.

Some portion of the stream would have to be purged to keep the inert level within acceptable limit.

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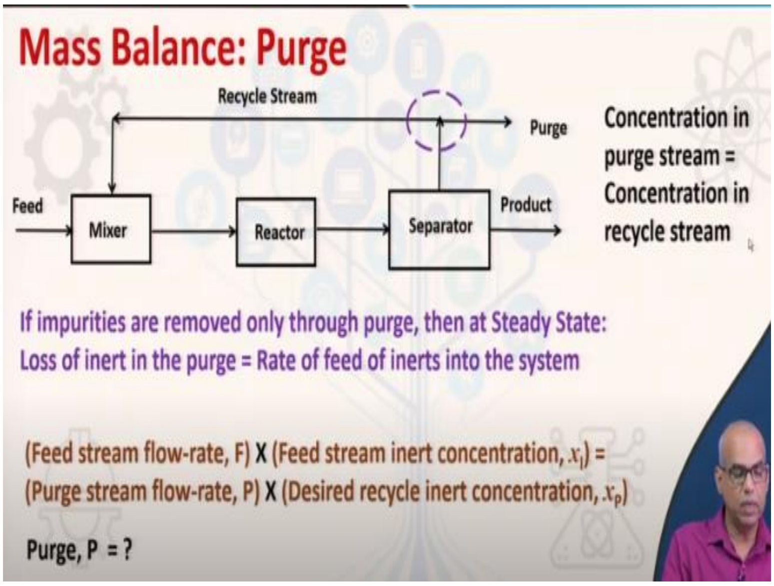


As the schematic shows the concentration in the purge stream will be equal to concentration in the recycle stream. If impurities are removed only through purge then at steady state you can write that loss of inert in the purge will be equal to rate of feed of inerts into the system. So this allows me to compute what will be the purge rate.

Because feed stream flow rate times feed stream inert concentration will be equal to purge stream flow rate times desired recycle inert concentration.

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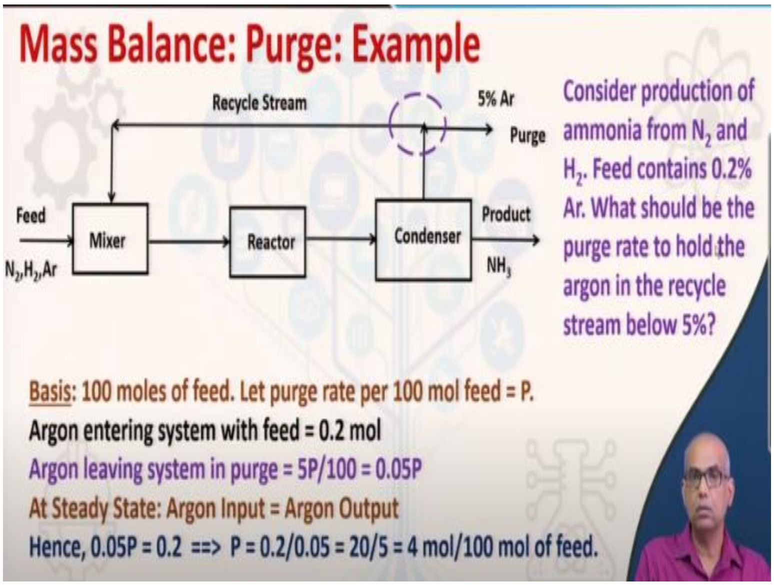


Let us solve a very easy problem. Consider production of ammonia from nitrogen and hydrogen. Feed contains 0.2% argon which is inert. What should be the purge rate to hold the argon in the recycle stream below 5%? Let us take basis 100 moles of feed. Let purge rate be 100 moles, let purge rate per 100 moles be P.

So how much of argon enters system with feed 0.2% so 0.2 mole. Argon leaving system in purge 5% so 5% of P is 0.05P. So you must equate 0.05P with 0.2. This gives me 4 moles per 100 mole of feed. So the purge rate should be 4 mole per 100 mole of feed.

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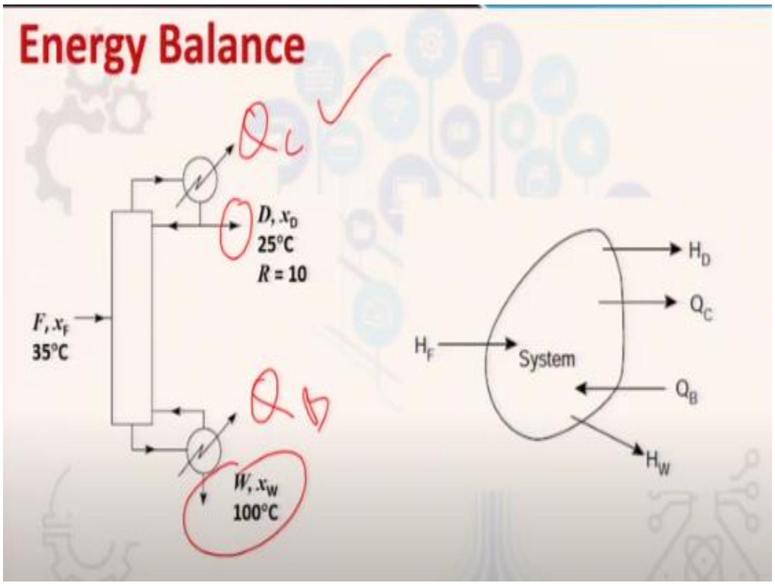


Finally, let us quickly talk about energy balance. What you see is a schematic of a distillation column. The feed with composition x F composition for the more volatile component and enters at 35 degrees Celsius. At the top the displayed rate is D. It may be given in terms of moles per hour or kilo moles per hour. Mole fraction or mole volatile component is x D. It is 25 degrees Celsius and reflux rate is 10.

The bottom product is withdrawn at the rate of W mole fraction x W temperature 100 degrees Celsius. Now the energy balance can be written similar to mass balances by defining system boundary. So let us try to identify the streams with which energy enters to the system and the streams with which energy leaves the system. So there are two streams through which energy enters.

One is feed stream. So enthalpy H F enters and another is Q B which is boiler load. So this is Q C and this is Q B. But energy leaves with the distillate. It leaves with condenser. It leaves also with the product stream at the bottom. So these are all the streams with which energy enters and energy leaves.

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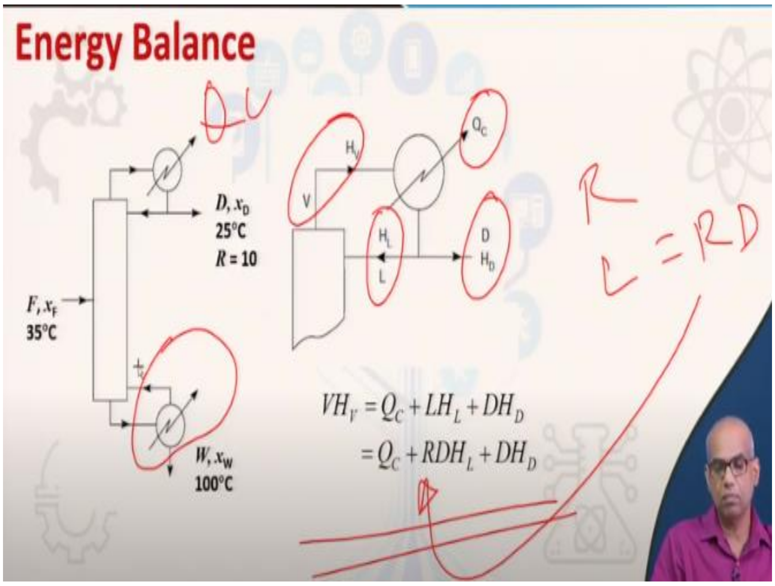


Now you can take appropriate system boundary and can write down energy balance equation. For example, let us consider the top part of the distillation column. So I can write energy balance around this envelope. So this is shown here. So you write energy balance around this envelope. So energy enters with H v energy leaves with this, this, as well as this.

So we can write v into H v the amount of energy that enters is equal to energy leaves L H L + D H D + Q C. Now reflux ratio is R. So you can use L = R D and can substitute here. So this will allow you to compute say Q C. Similarly, you can write energy balance around this envelop. You can also take an envelop around the entire distillation column and can write energy balance equation.

So you have to identify the streams with which energy enters and you have to identify the streams with which energy leaves. And then at steady state, energy balance can be written the same way as we have seen in case of mass balance energy in equal to energy out. So with this, we stop our discussion here. Thank you for watching.