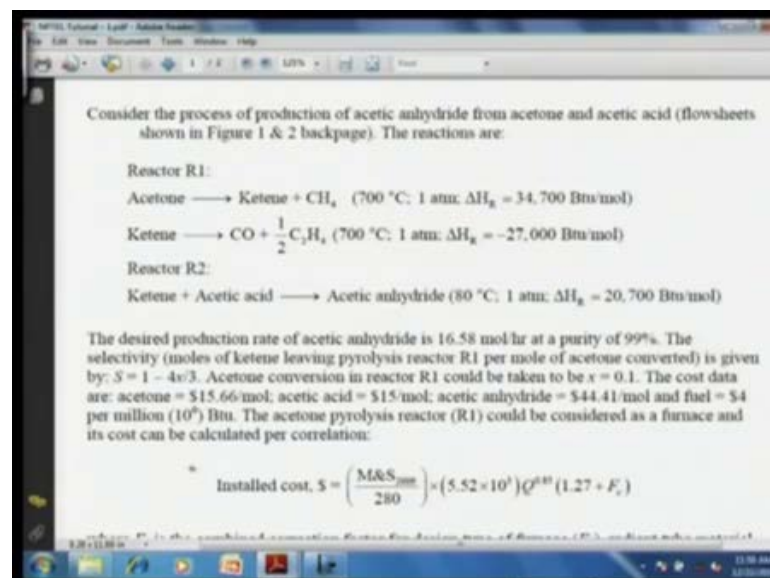**Process Design Decisions and Project Economics**
Prof. Dr. V. S. Moholkar
Department of Chemical Engineering
Indian Institute of Technology, Guwahati

Module - 2
Flow Sheet Synthesis
(Conceptual Design of a Chemical Process)
Lecture - 12
Tutorial (Part III)

Welcome, in the previous tutorial of the module of flow sheet synthesis, we saw as how we can develop the input output structure of a flow sheet from the basic reaction given and also determine the material balance. Next is determination of the recycle structure of the flow sheet and the corresponding material balance. Some basic calculations about the reactor area and the heat load for the taking isopropanol decomposition to acetone as the case study. In this tutorial, we go one step ahead and try to determine the exact economic potential of a particular process at various levels of the design, that is the input output structure and recycle structure.

(Refer Slide Time: 01:20)

Here, we take the example of acetic anhydride manufacture from acetone and acetic acid. I have already given this example in the one of the previous lectures of this module, when we dealt with the number of reactor systems. What you see on the screen now, is the problem statement. Consider a process of production of acetic anhydride from

acetone and acetic acid. The basic reactions are in the first reactor, acetone decomposes to species called ketene and methane at temperature of 700 degree centigrade, pressure of 1 atmosphere. Since, this is a decomposition process, it is endothermic and the heat of reaction is 34,700 Btu per mole of acetone.

The ketene is an unstable species, which can further decompose to carbon monoxide and ethylene. This side reaction also occurs at the same temperature and pressure, but since it is a composition, means it is a dissociation process. It is exothermic and the heat of reaction is minus 27,000 Btu per mole. This particular stream enters the second reactor in which acetic acid is added and acetic acid reacts with ketene to give acetic anhydride. The second reactor however, operates at a much lower temperature of 80 degree centigrade and atmospheric pressure.

Here, the heat of reaction is 20,700 Btu per mole. We take the desired production rate of acetic anhydride as 16.58 moles per hour with a purity level of 99 percent. The selectivity moles of ketene leaving pyrolysis reactor 1 per mole of the acetone converted; is given as S is equal to 1 minus 4 x by 3. So, the selectivity is a function of conversion. The acetone conversion in the first reactor we have, we can take as about 10 percent. The cost data is acetone 15.66 dollars per mole, acetic acid 15 dollars per mole, acetic anhydride 44.41 dollars per mole. Fuel cost is dollar 4 per million Btu.

The acetone pyrolysis reactor could be considered as a furnace. Its cost can be calculated using a cost correlation. Now, cost correlations, we are going to see in detail in another module. To determine cost of any equipment of a process, a correlation is used, which uses one of the specific characteristics of that particular equipment as parameter. Now, since the reactor is considered as a furnace, the heat duty Q is taken as the characteristic parameter. The cost correlation is installed cost in dollars as M and S 2009 divided by 280. Now, these are the cost indexes.
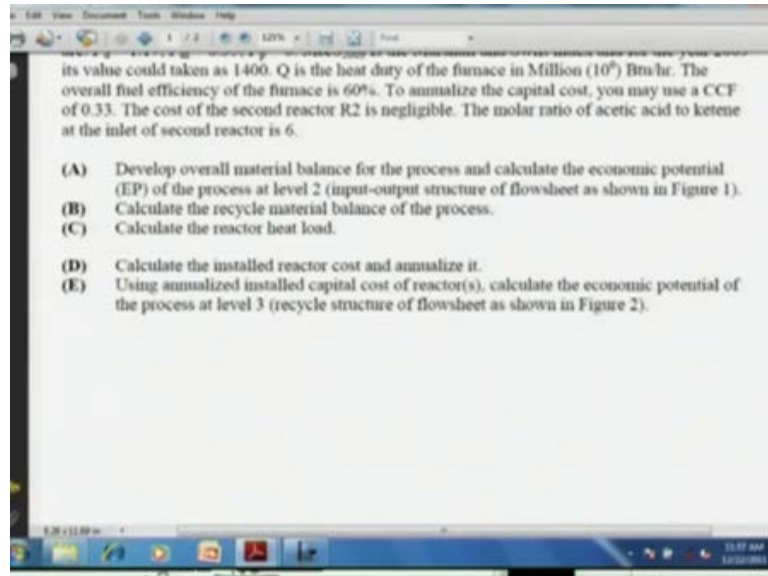
When the cost correlation was proposed, the index was 280. Now, at in 2009, the Marshall and Swift index is given to be 1400 into this cost index into 5.52 into 10 to power 3 into Q, which is the heat load in mm Btu, million metric tons million metric Btu. Q rests to 0.85 into 1.27 plus F c, where F c is the combined correction factor for the designed type of furnace. Now, designed type of furnace, the correction factor is F d, the radiant tube material and a design pressure and a total correction factor. Because of these three types, the design type of a furnace the tube material and a design pressure is just a summation F c is equal to F d plus F m plus F p.

The values of the correction factor are 1.17, 0.35 and 0 for F d, F m and F p respectively. I just said that Marshall and Swift index, you can take for 2009 as 1400. Q is the heat duty of the furnace in mm Btu. The overall fuel efficiency of the furnace is 60 percent. Now, in order to determine the economic potential of the process, we have to annualize the capital cost. Now, there are some costs of this particular process which are of recurring time, which means we have to pay them annually.

Some costs are single time cost like for example, the capital cost of the reactors. So, in order to determine the economic potential, these two costs have to be brought on the same basis. So, what we do is that, we annualize the capital cost. Now, how is this done? We shall see in detail in the next module, but here, I just give an introduction that the annualization of the capital cost can be done using a parameter called capital charge

factor the CCF which is typically 1 by 3 or 0.3. The cost of the second reactor is negligible because it is simple addition. So, that we do not take into consideration. The molar ratio of acetic acid to ketene at the inlet of second reactor is taken to be 6.

(Refer Slide Time: 07:11)

its value could taken as 1400. Q is the heat duty of the furnace in Million (10^6) Btu/hr. The overall fuel efficiency of the furnace is 60%. To annualize the capital cost, you may use a CCF of 0.33. The cost of the second reactor R2 is negligible. The molar ratio of acetic acid to ketene at the inlet of second reactor is 6.

(A) Develop overall material balance for the process and calculate the economic potential (EP) of the process at level 2 (input-output structure of flowsheet as shown in Figure 1).
(B) Calculate the recycle material balance of the process.
(C) Calculate the reactor heat load.

(D) Calculate the installed reactor cost and annualize it.
(E) Using annualized installed capital cost of reactor(s), calculate the economic potential of the process at level 3 (recycle structure of flowsheet as shown in Figure 2).

We have to answer several questions. First is developing of the overall material balance for the process as we did in the previous module and calculate the economic potential of the process at level two, the input output structure. Now, in the figure that I will show, this flow sheet will be shown. Now, calculate the, calculation of the recycle material balance of the process and then calculation of the reactor heat load; then determination of the installed reactor cost and annualizing it. Finally, using the annualized capital cost and the other cost, the cost of all the other process flows, calculation of the economic potential of the process at level three, that is the recycle structure of the flow sheet.

(Refer Slide Time: 07:58)

Figure 1: Input-Output Structure of Flowsheet (Level 2)
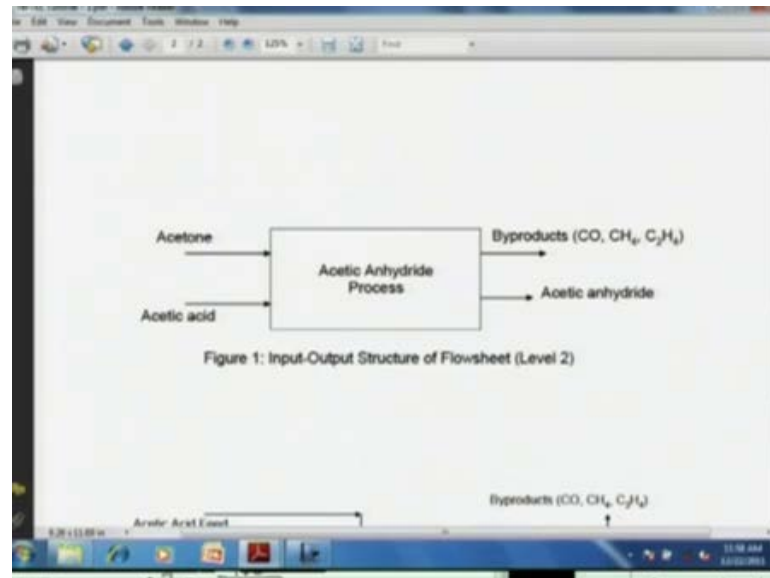
Now, let us see the input output and a recycle structure before we proceed with the calculation. The input output structure is now on your screen that is, level two. We have a process. The two feed streams are acetone and acetic acid. Then the main product that comes out is acetic anhydride. Then the byproducts that are carbon monoxide and ethylene generated due to the dissociation of ketene and methane that is due to the decomposition of acetone to ketene. So, this is a simple input output structure of the flow sheet. The recycle structure of the flow sheet is now on your screen.

Figure 2: Recycle Structure of Flowsheet (Level 3)
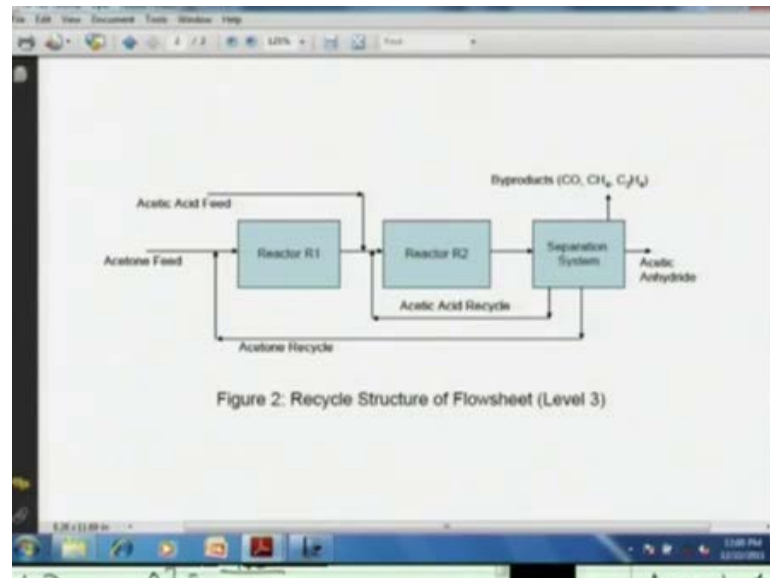
What we have is the system of two reactors. Now, since the reactions are occurring at significantly different temperatures, we cannot have them in the same reactor. The first reaction of acetone composition is at 700 degree centigrade while the second reaction of addition of ketene to acetic acid is at only 80,70 degree centigrade, 70 or 80 degree centigrade. So, because of this difference of temperatures, we cannot have both reactions in the same reactor.

So, we need two reactors. The separation system would try to separate out the main product, acetic anhydride and also the byproducts carbon monoxide, methane and ethylene which could be further used as fuel in the same process, at some other equipment. Then the two recycle streams will be generated from the separation system. First is the unconverted acetic acid and second is the unconverted acetone. However, acetic acid and acetone are fed to two different reactors.

So, we will have to have two recycle streams. Remember, not single recycle stream as incase of previous example of acetone manufacture through IPA, a dissociation or a dehydration of IPA, isopropyl alcohol. Here, you will have two recycle streams. The acetic acid recycle will go at the inlet of reactor two. Acetone recycle stream will go at the inlet of reactor one. So, this is a simple recycle structure that we can generate from the basic chemistry, that is given or the basic process considerations. We start with our calculations.

First, the material balance at input output structure of the flow sheet or the level two. We have been given the desired production rate of acetic anhydride that we not by ACAN, as 16.58 mole per hour. Now, from stoichiometry, we can write easily the consumption of acetic acid also to be 16.58 moles per hour. Now, the selectivity in the present situation is the function of conversion 1 minus 4 x by 3 and conversion is taken to be 10 percent. So, by substituting x equal to 0.1, we can get the selectivity as 0.87. The acetone that is converted will be the production rate of acetic anhydride, that is, main product divided by the selectivity. So, 16.58 divided by 0.87 that is 19.o6 mole per hour.

Now, from stoichiometry, we can easily calculate production rate of methane also, as 19.o6 mole per hour. The ketene that is lost through dissociation to carbon monoxide and ethylene will be obviously PACN, the production rate of acetic anhydride into 1 minus s divided by s, that is 2.48 moles per hour. Production rate of Carbon monoxide will be same as this due to stoichiometry, 2.48. Production rate of ethylene will be half of this, again due to stoichiometry.

So essentially, we have determined the flow rates of all the components in the level two. Now, the gas byproducts, carbon monoxide, methane and ethylene can be captively consumed as fuel in the process. Now, we have to determine the fuel value. But, before we do that, we have to see the heat of combustion of these gases. For methane, the heat of combustion is minus 0.761 million Btu per mole, for ethylene, minus 1.254 Btu mm million Btu per mole. For carbon monoxide, it will be minus 0.268 mm Btu per mole. The fuel cost in general, can be taken as 4 dollars per m m Btu. This is the same value as we have used in our previous example of acetone manufacture.

(Refer Slide Time: 15:29)

Now, given all these information, how we can write the economic potential at level two; that is input output structure of the flow sheet. The economic potential per hour basis will be the value of acetic anhydride. The main product minus the values of the two reactants, value of acetic acid and value of acetone plus the cost of the energy that we recover through combustion of the gas gaseous side product; that is the fuel value of COCH4 and C2H4.

Now, we have been given all the cost. Acetic anhydride is 44.41 dollars. So, all that things, all those numbers we add. This was the cost of acetic acid. Now, cost of acetone into the consumption of acetone; that is 19.06 mole per hour and plus the heat that we are going to recover through carbon monoxide, acid ethylene and methane. This is for methane. This is for carbon monoxide and this is for ethylene. This is mm Btu per hour into dollar per mm Btu. So, what we have, if you now simplify this, what we have is dollar 256.04 per hour. This is the economic potential at level two. Now, this is per hour. The annual potential will be this into 8000 hours per year which will be something like 2 million dollars annually. So, the economic potential is positive, which means the process is profitable.

(Refer Slide Time: 19:54)

So, we go to the next level that is the determination of the recycle structure of the flow sheet. This is the level three of design. Now, here again, we have to the material balance. There are two recycle streams as I mentioned to you before the acetone recycle and acetic acid recycle. So, then we first see the acetone recycle. The total feed rate of acetone to the process will be F acetone, the F acetic anhydride by x, then the unconverted fraction. So, 19.06 divided by 0.1 into 0.9. Sorry, I am this is wrong.

Please make correction. The acetic recycle will be the total acetone, F F acetone, the fresh acetone fed to the process divided by x and then into 1 minus x. So, this is the total acetone feed, which the fresh acetone is divided by x. Then this is the unconverted fraction. Now, we assume 100 percent recovery. So, by substituting values, we get the recycle acetone as 171.54 moles per hour. Now, the acetic acid, we have been given the molar ratio of ketene and acetic acid. Acetic acid is added in excess.

So, the molar ratio is 6. Now obviously, we assume complete conversion of ketene, which is unstable species. So, the recycle acid will be the excess acid that is added. The number of moles of ketene that enter reactor are 16.58 out of which, due to stoichiometry 1 mole reacts with 1 mole of ketene reacts with 1 mole of acetic acid and an unconverted fraction is the excess acetic acid, which is 82.9 mole per hour. So, this is how the material balance for the recycle streams.

(Refer Slide Time: 23:42)
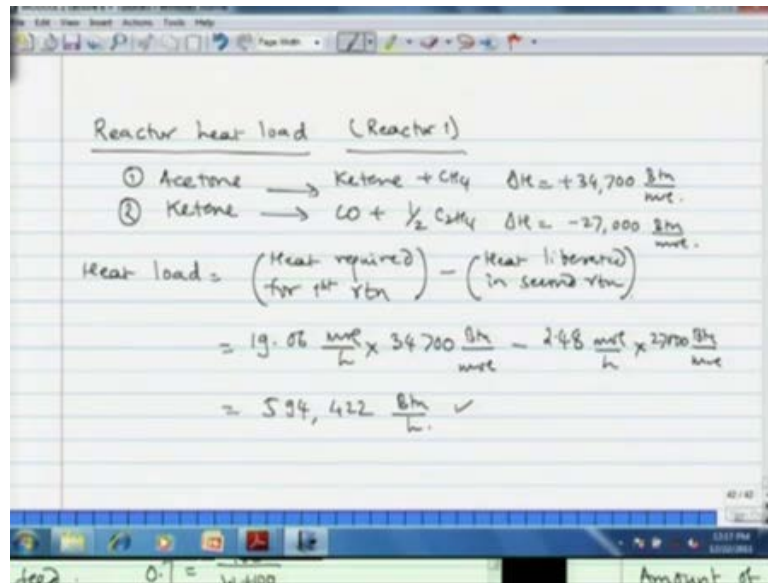
Now, the next question is about determination of the reactor heat load. Now, reactor heat load is essentially for reactor one. For the second reactor, reaction occurs only at 80 degree centigrade. Reaction is rather fast due to unstable nature of ketene. Therefore, there is not much heat load there. But, for the reactor one, we have significant heat load due to the decomposition. Now, here two reactions occur.

First is the decomposition of acetone to ketene and methane and then dissociation of that unstable species ketene into carbon monoxide and ethylene. The first reaction here is exothermic. Sorry, the first reaction is endothermic. Acetone decomposing to ketene plus methane is endothermic with delta H of plus 34,700 Btu per mole. Side reaction of dissociation of ketene to carbon monoxide and ethylene is endothermic with delta H as minus 27,000 Btu per mole.

Given these heat of reaction and the material balance that we have just obtained, we can easily calculate the heat load. The heat load will be the heat required for first reaction, acetone decomposing to ketene, methane minus the heat liberated in second reaction. 19.o6 per hour of acetone are decomposing with heat requirement of 34,700 Btu per mole minus 2.48 moles of ketene, that are last liberating 27,000 Btu per mole. So, the net heat load is 594,422 Btu per hour. Now, this much heat has to be supplied to the reactor. Now, reactor, we consider as a furnace.

So, the heat duty is what we just determined. Now, we have to get now installed reactor cost. We have been given a correlation. Installed cost is in dollars is equal to the cost index. Now, this is for year 2009. You can easily update it to 2011 or 2012, by looking into techno commercial journals like chemical engineering journal or chemical industry digest chemical weekly. This cost indexes are published annually in these techno commercial journals.

The correlation was proposed in 1969. So, the cost index in that year is 280. So, we multiply to update the cost. We multiply by the ratio of these indexes. The heat duty Q rests to 0.85 plus all the correction factors. F c, correction factor is the summation of correction factor due to design, due to the material of tubes or material of construction and the operating pressure. We have been already given the values.

So, we simply substitute to get the net correction factor; 1.17 plus 0.35 plus 0 that is 1.52. Now, we substitute for Q that we just determined. Now, this Q is in Btu per hour. So, in mm Btu, 3.594 mm Btu because the heat loads in the cost correlation is in million metric Btu. Cost index is 1400 divided 280 into 5.52 into 10 to power 3 into 0.594 rest to 0.85into 1.27 plus 1.52, the correction factor. So, we get cost, installed cost as 49,473 dollars. Now, this is the single time cost. It is like capital cost, single time cost. We have to annualize it. The annualized cost will be the installed cost into CCF.

(Refer Slide Time: 29:29)

So, the annualized cost is dollar 49,473 by 3 plus CCF is 1 by 3 or 0.33. What we are getting and that comes out to be 16,491 dollars per year. So, this is the installed annualized capital cost for the furnace. We have to determine the operating cost of this furnace. The operating cost will be nothing but the fuel cost for furnace plus maintenance and repair etcetera that we ignore.

The fuel cost of furnace will be the total heat duty into number of operating hours; total heat duty per hour into number of operating hours into the fuel cost divided by the efficiency. Now, we substitute all values that we have. The efficiency is given to us as 60 percent. The total heat load that we have already calculated 594,000 Btu into 8000 hours per year into fuel cost that is dollar 4 per m m Btu million metric Btu. So, we have to now here multiply by 10 to power minus 6 to convert Btu to m m Btu divided by 0.6. Then if you just calculate, you will get the fuel cost as 32,286 per year. This is the annual fuel cost.

Therefore, the total cost for the reactor or the total annual cost for the reactor is equal to the annualized capital cost plus the annual fuel cost. At numbers, we already have we just substitute annualized capital cost was 16,491 dollars plus this cost, 32,286 dollars. So, total 48,777 dollars per year. Now, having done these calculations, we have to now determine the economic potential of the process at level three. Now, this EP, economic potential at level three is EP 2 minus the annualized capital cost of the reactor, total annual cost of reactor. The EP 2, economic potential at level two, we had already seen here as 2, 86,687 dollars.

Now, we have to simply deduct that particular hmm the annualized cost of process. For, we take this 407, so approximate value. After adjusting these figures to the nearest integers like 48,777 we adjust to 49,000 and 286,000 that we do. By doing all these things, we can get the annual economic potential at level three as 2, 00,000. This we adjust as 49,000, so 86 minus 49 that is 7,237,000 dollars.
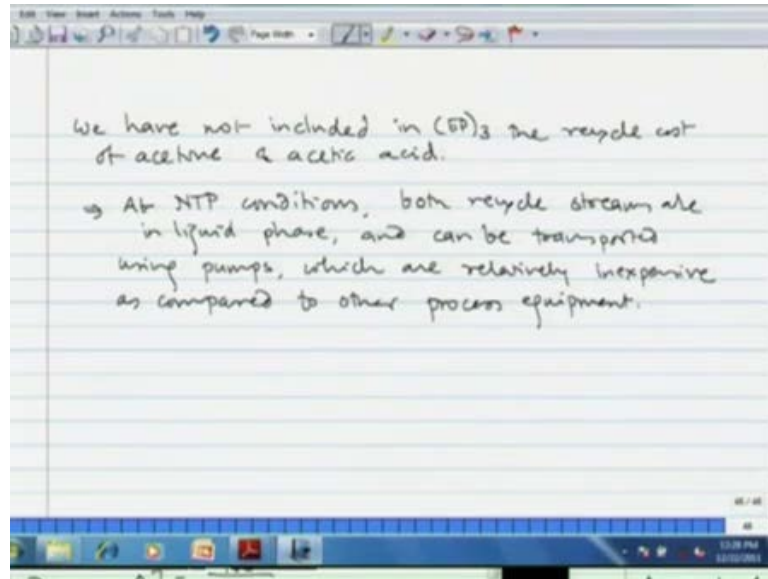
One important point we have not included here while calculating this economic potential. We have not included the recycle cost of acetone and acetic acid. However, you can easily note that both acetone and acetic acids are liquids at NTP conditions. So, you will require simple pumps for recycling them. The cost of pump is rather negligible as compare to the other cost that we have seen.

Therefore, we have not included here the cost of the recycle streams. That point we note. At NTP conditions, both recycle streams are in liquid phase and can be transported using pumps, which are relatively inexpensive as compared to other process equipment. Therefore, we do not include these minor details in our analysis. So, this is how you can generate the economic potentials at various levels. Now, we have seen that both economic potentials were positive, economic potential at level two and level three.

Therefore, it justifies the additional effort for the detailed design of the process especially the reactor and also the separation steps. Continuing with the same theme, we shall see another problem in which we shall determine the economic potential of the HDA process with design variables. Now, we are very well aware with the hydro dealchylation of HDA process because that we have used as a model throughout our module.
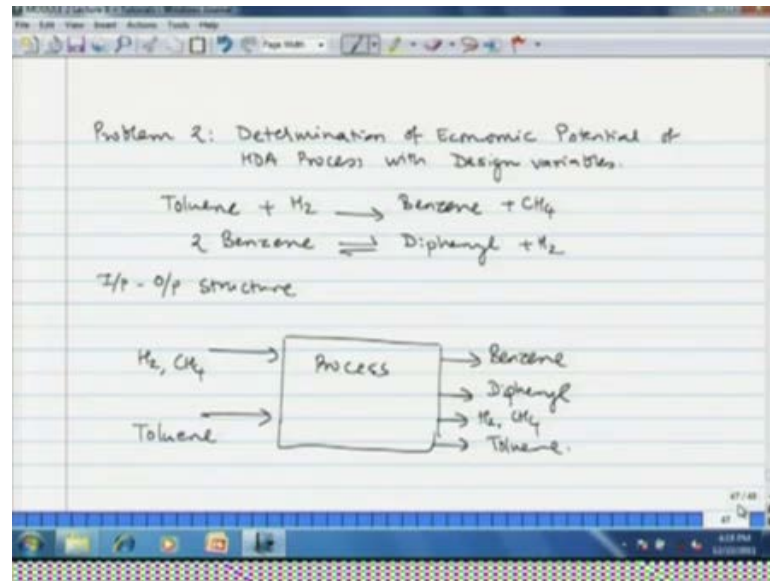
The basic reactions are toluene reacts with hydrogen to give benzene and methane. There is side reaction of two molecules of benzene combining to form one molecule of diphenyl and hydrogen. Hydrogen always contain some impurity of methane because hydrogen is generated through steam reforming of methane. Toluene can be assumed to be pure. So, the input output structure of the flow sheet is the process with hydrogen and methane as with impurity of methane as the gas of feed stream, toluene as liquid feed stream. There are five streams coming out benzene, diphenyl and hydrogen with methane that I have shown together and toluene. The recycle structure of the flow sheet is also well known to us.

(Refer Slide Time: 38:40)
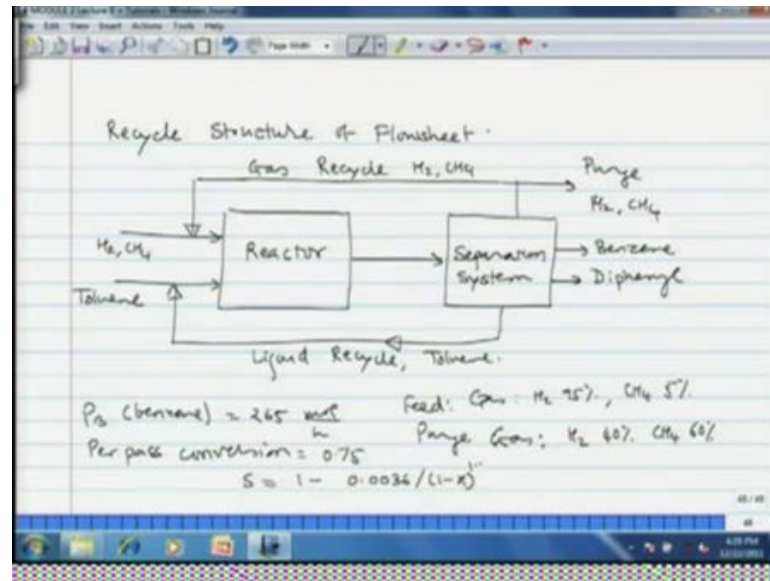
We have seen it several times before, the process with input of hydrogen and methane, toluene as the main limiting reactant. Hydrogen is fed in excess following the process, there is following the reactor, not process, following reactor, there is a separation system comprising of flash drum and distillation column. Benzene and diphenyl are separated as main product and byproduct. The unreacted toluene is recycled. The gas that comes out is split in two parts. Some part is purged and another is recycled. So, that is the recycle structure of the flow sheet.

Now, let us give some numerals. Let us say the production rate of benzene is 265 mole per hour. The per pass conversion of toluene is 0.75 feed. Toluene is assumed to be pure. Hydrogen contains 5 percent methane as impurity. Purge composition, purge gas contains 40 percent hydrogen and 60 percent methane. The selectivity is a function of conversion and is given by this correlation. S is equal to 1 minus 0.0336 into 1 minus x rest to 1.544.

Now, the cost data; cost data, the price of benzene can be taken as 9 dollars and 4cents per mole. Price of toluene 6.4 dollars per mole hydrogen means, we as say this make up gas which includes methane as impurity, can be taken as dollar 1.14 per mole. The fuel cost is dollar 4 per million Btu. The fuel values of various components are hydrogen 0.123 million Btu per mole, methane 0.383 MMBTU per mole, benzene 1.41 million Btu per mole, toluene 1.68 million Btu per mole and diphenyl 2.688 million Btu per mole.

Having given this data, we have to first determine the material balance for the process, both for input output structure as well as the recycle structure. Now, we have done this before in I think the second or third lecture of this module. So, what I will do that instead of repeating the same calculations again, I will directly give you the expressions. You can go back to the lectures and see as how these have been derived. So, that it is left as an exercise the revision.

(Refer Slide Time: 42:55)

I am directly giving the equations. Now, material balance; I am giving in terms of the variables. We can put the numbers later. The fresh toluene feed which we denote as FFT will be equal to PB by S where S is selectivity which we have been given as 0.0366 divided by 1 minus x rest to 1.544. Then methane generated in reaction that we denote as PRCH4. This is also same as PB by S due to stoichiometry. Amount of toluene lost to diphenyl, which FFT into 1 minus S by 2. So, that is a production rate of diphenyl, which we can now write in terms of production rate of benzene as PB by S into 1 minus S by 2.

Now, we have already derived expressions for the purge gas PG is equal to FG, fresh gas plus PB by S into 1 minus S by 2 and the fresh gas FG is PB by S into 1 minus YPH. YPH is the mole fraction of hydrogen purge gas into 1 minus S by 2. This whole thing divided by YFH minus YPH where AYFH is the mole fraction of hydrogen in fresh gas, which has been given to us as 0.95.

(Refer Slide Time: 45:11)

We substitute the values in these expressions. The selectivity S is 1,1 minus 0.0036 divided by 1 minus x rest to 1.544. Now, if you substitute x is equal to 0.75 that is the per pass conversion, then we get S is equal to 0.9694. The fresh feed rate of toluene will be PB by S which is 265 divided by 0.9694 which turns out to be 273.4 that we approximate at 273 moles per hour, then the diphenyl production, PB by S into 1 minus S by 2. So, again putting all values, we get diphenyl production as 4.18 moles per hour, which we can approximate as 4 moles per hour.

Then, the makeup gas FG again, we put all values 265 into 1 minus 1 minus 0.4 into 1 minus 0.9694 whole divided by 2. This divided by 0.9694 into 0.95 minus 0.4. So, this is 492.5mole per hour. Purge gas is 492.5 plus 265 into 1 minus 0.9694 divided by 2 into 0.9694, is equal to 496.7 moles per hour.

(Refer Slide Time: 47:43)

Now, the economic potential; we have not considered the recycle structure. Therefore, economic potential at level two will be value of benzene plus fuel value of diphenyl. Because diphenyl once removed is used as fuel plus the fuel value of purge gas minus the value of toluene, the value of makeup gas, the two feed streams. Now, if you put all values here, if you put value of benzene as 265 into 9.265 moles per hour into dollar 9.o4 per mole fuel cost of diphenyl, that is 4.18 mole per hour into the fuel value 2.69 m m Btu per mole.

Then, cost of purge YPH which is 0.4 into the purge gas, which is 496.7 moles per hour into the fuel value of hydrogen plus the fuel value of methane. Now, minus the cost of toluene that is 273 mole per hour into dollar 6.4 per mole plus the makeup gas, which was 492.5 mole per hour into dollar 1.14 per mole. Then if you do this then you get the economic potential as dollar 683.9 per hour. Then assuming 8000 hours per year, the total annual economic potential will be 683. You can take as 684 into 8000. That turns out to be 5.4 million dollars, 5.46 million dollars. So, this is how you can calculate the economic potential. Now, let us change the design parameter slightly.

(Refer Slide Time: 51:15)

Let us say, that for YPH equal to 0.1 and per pass conversion as 0.5. What are the variables or what is the economic potential? Then we can easily calculate all the parameters. Now, you can make an excel sheet of this or a math card sheet. You can take care at a make any module and then you can calculate these values. I am giving directly the answer. I leave the exact calculation as an exercise. For YPH equal to 0.1, that means we are essentially purifying the gas stream that is coming out of the flash drum.

So, only 10 percent hydrogen is lost through the purge gas; everything else is recycled. So, you use the same formula that I have listed earlier. Then I will give the answer. It comes out to be 0.99. FFT comes out to be; fresh toluene comes out to be 267.8, diphenyl 1.4 moles per hour. Then fresh gas is reduced because of purification of hydrogen, for 313.5 moles per hour. Purge gas as 314.9 moles per hour. Then if you substitute all values of cost then the economic potential at second level turns out to be 789 dollars per hour. You can see a rise of economic potential as you purify the gas stream that means very little hydrogen is lost in the purge stream. Everything is recycled. So, this is how you can easily make calculations for economic potential.