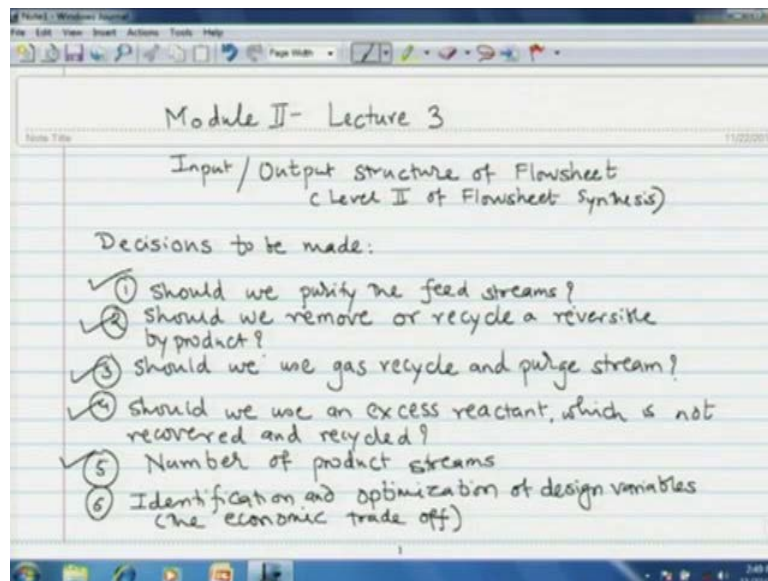


Process Design Decisions and Project Economics
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Module - 2
Flowsheet Synthesis (Conceptual Design of a Chemical Process)
Lecture - 6
Input / Output Structure of Flowsheet (Part II)

We are now in the module 2 of our course, which is Flowsheet Synthesis. In the previous two lectures, we saw the hierarchical approach to flowsheet synthesis, the hierarchical approach essentially consists of 5 steps. In the first step we have to decide, whether we want to go for a batch process or continuous process, in the second step or level 2, we have to decide the input output structure of the flowsheet. In step 3 we have to decide the recycle structure of the flowsheet, in step 4 we have to design the separation systems in the process, and finally in step 5 we have to do the energy integration of the process.

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We have already seen the decisions for the batch process, continuous process, under what circumstances we go for batch process, under what circumstances a continuous process is preferred. In previous lecture, we started with level 2 of the flowsheet synthesis, that is input output structure of the flowsheet, we have to make basically 6 decisions.

In this stage or level 2 of the flowsheet synthesis, the first decision is we have to see, whether we have to purify the feed streams. After selecting the process, after knowing the basic chemistry of the process, we have to start designing the process and the first question is that of the feed stream; and then we have to see whether we have to purify the feed streams.

Then the next decision is about removal or recycle of a reversible byproduct, rarely there will be a process with only single product. There will always be several side product reactions taking place, giving rise to several unwanted byproducts. Now, if some of these byproducts are formed through reversible reactions, we have to decide whether we have to remove these byproducts or recycle.

Then, the third decision is about gas recycle and purge now, several impurities enter with the gas feed streams or several gaseous products are also generated in the system. If we recycle all the unreacted gaseous reactant, then these innards or byproducts also get recycled and they get accumulated in the process, which will hamper the smooth operation of the process.

Therefore, we have to use a purge stream where, we will throw off some of the unreacted reactant so as to, throw off the impurities or innards also with these streams. The remaining stream has to be recycled, however gas recycle is associated with higher cost, because of the gas compression. And therefore, gas recycle streams form a significant cost component of the process.

Then the next decision is that, whether we should use an excess reactant and whether we are to recover this unreacted excess reactant at the end of the process. The example that we saw was that of combustion process, in which excess air is fed now, air being free we never try to recover air. However, there is a limit to this excess reactant, if you go on feeding larger and larger amount of air, then the cost of blower a compressor goes up for handling such large air streams.

Then, the next decision was about the product streams, how many product stream there should be. Now depending on, what is the fate of the product that is coming out of the process, we decide the product stream. The thumb rule that we used for this particular decision was that, never separate and mix two streams if their destination is same. For

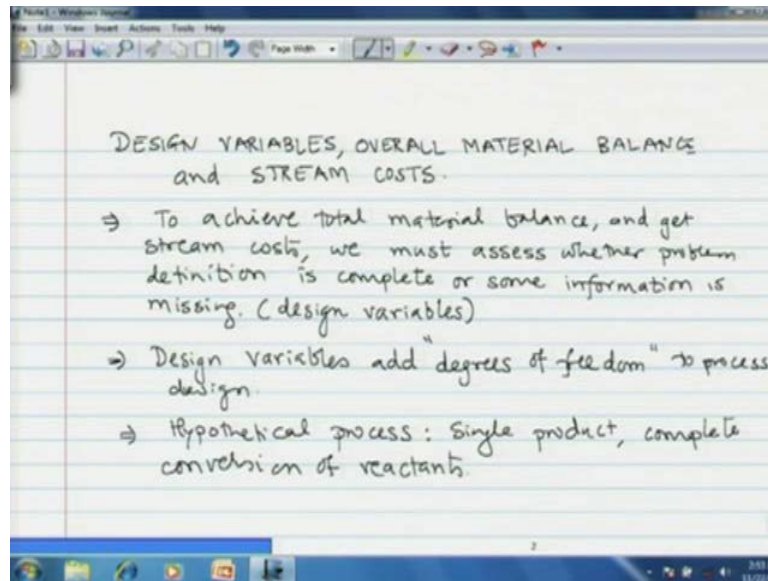
example, if there are unreacted liquid reactant, then if there are more than one such reactant then it is not necessary to separate them.

You can recycle in the same stream such that, although the reactant or components are more than one, the stream, the product stream is a single stream. Then there was another criteria that was associated with deciding product stream is that of the feeds of that particular component. We listed all the components in the increasing ascending order of their normal boiling point and then we grouped those reactants, which were in the vicinity of their boiling points and where the destination was also same.

For example, in the HDA process, we hydrogen and methane through same recycle stream so the product stream is single, although the components are two. Why, because hydrogen and methane both are gases and both either go to purge or they go to recycle. So, that is how, we decide the number of product streams and finally, we have to do the overall material balance.

And then we have to identify certain design variables now, as I mentioned in the very first lecture, the process design problems are always under defined. That means, not all of the information that is required to design the process or even to do the complete material or energy balance would be available. In such cases, we have to make the use of thumb rules to get the missing information or we have to look into the literature where, similar or same process has been treated or we can simply use our own experience to guess the missing data. We have already seen the first 5 decisions in previous lecture, so now we go for the 6th decision that is, identification and optimization of design variables.

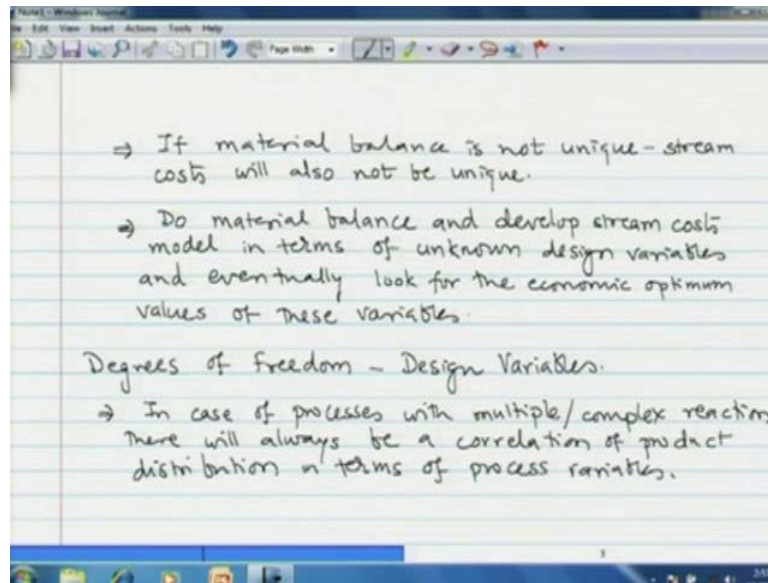
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Design variables, overall material balance and stream cost that will be the topic of today's discussion. To achieve total material balance of the process, we have to have the complete problem definition however, as I just mentioned, the problems are under defined and some data is missing, that point we note. To achieve total material balance and get stream cost, that will help us identify the economic potential of the process, we must assess, whether problem definition is complete or some information is missing.

This information could be in terms of design variables, that we will now just see and these variables add the degrees of freedom to the process design. Now, consider hypothetical process, in which there is a single product generated from one or more reactants and the conversion is complete. Now in such cases, there is no freedom of designing a process, you start with direct material balance based on stoichiometry designing reactor. So, such hypothetical process has zero degrees of freedom, for such process there will be unique set of material balance, unique set of energy balance and the reactor design is based on that. However, in most of the processes the product is not same, multiple products are there, the product distribution depends on conversion, temperature, pressure so on and so forth. And all these parameters add degrees of freedom to the process so that point we also note.

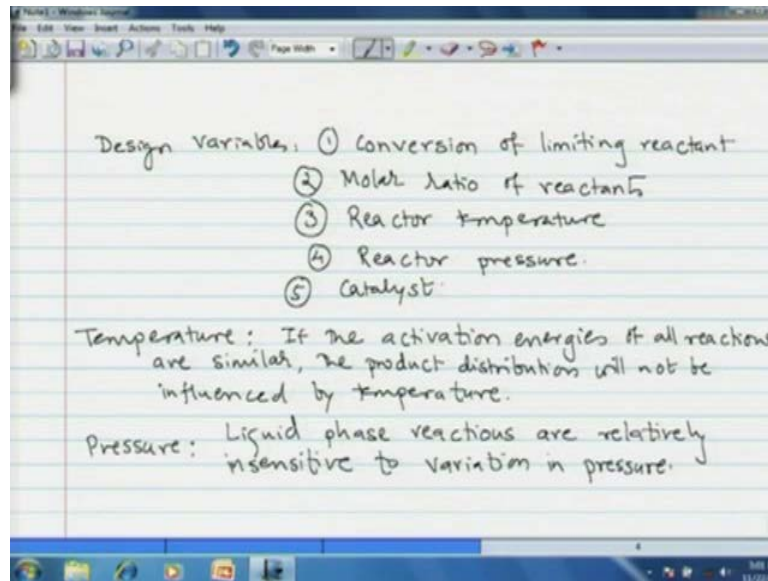
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If the material balance is not unique, stream cost will also not be unique and therefore, we have to do the material balance or develop the stream cost model. And once, we develop such a model then we have to do the optimization studies, this eventually look for the economic optimum values of these variables. Now, we shall see the application of these principles with an example, before we do that let us see, what are the degrees of freedom or what are the design variables, that we can have.

In case of complex reactions or processes that involve multiple reactions, there will always be the correlation of distribution of the products, in terms of the process variables. So, that point we note, in case of processes with multiple or complex reactions, there will always be a correlation of product distribution in terms of process variables or design variables, that we can also say.

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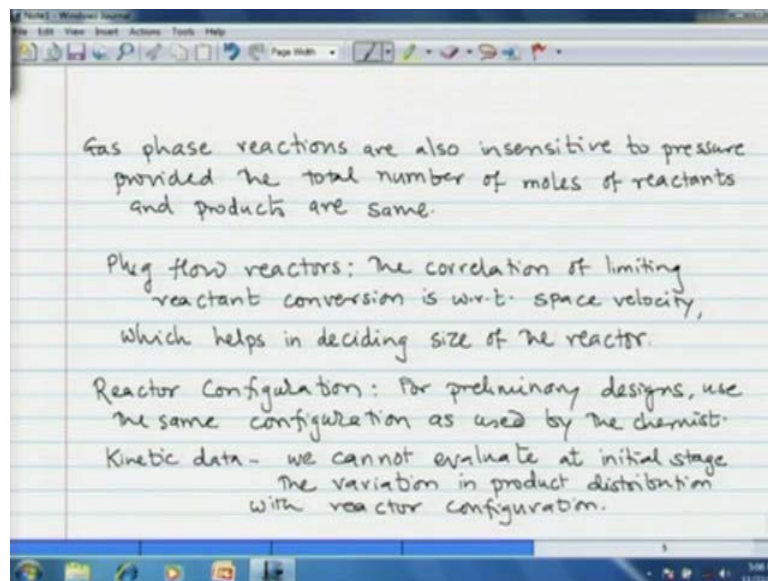


Now, what are these design variables, 1st is the conversion of limiting reactant then next is the molar ratio of reactants, 3rd would be the reactor temperature, 4th will be the reactor pressure and in case of catalytic reactions, the catalyst that is used. But now, we shall see what are these variables, that are significant and under what circumstances, they become insignificant.

As far as temperature is concerned, the rate of any reaction increases with temperature and that increases proportional to the activation energy. However, if the activation energies of all the reactions are similar or same then temperature will not appear in the correlation. So, that point we note, if the activation energies of all reactions are same or similar, the product distribution will not be affected by variation in temperature, because rates of all reactions that lead to different products, will vary almost same with temperature.

The reactor pressure, liquid fed systems are not so sensitive to variation in pressure so if the phase of the reaction is liquid, then it is unlikely that pressure will affect the product distributions significantly. Even in case of gaseous reactions, pressure will not matter, if the number of moles of the product as well as reactant are same. So, that point we note, liquid phase reactions are relatively insensitive to pressure because liquid properties are relatively insensitive to pressure. I am using the word relatively because in case of very high pressure, there could be a significant effect.

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Obviously, if the number of moles are reducing from reactant to product, high pressure will have increased conversion. If the number of moles are reducing then low pressure will favor higher conversion. In case of plug flow reactors, the correlation of reactant conversion that is mainly the limiting reactant conversion is with respect to the space velocity now, this helps in deciding the size of the reactor. Now, taking the same stream

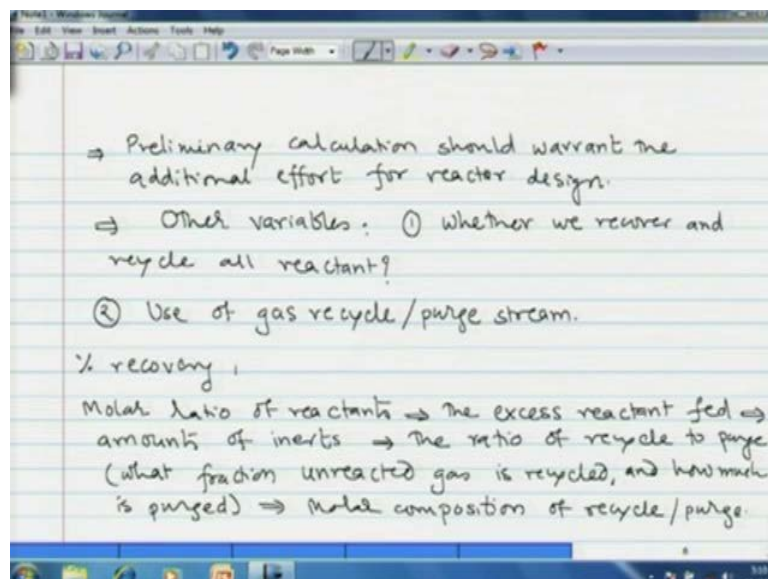
further, we have to see, as which reactor configuration will suit most for a particular reaction, whether we should go for a batch reactor or a continuous flow reactor, that is a basic distinction.

Now, in case of solid fluid reactions, we have options of having of fixed bed reactor or moving bed reactor, a fluidized bed reactor. Now, in fluidization also we can have different modes of fluidization, whether bubbling mode or turbulent mode or continuous circulating fluidized bed mode so on and so forth. Now, when we are at the very initial stage of the design, going into such complexities is not possible because of, lot of information that is needed for making such decision.

So, the best idea would be, for initial stages of the design, consider the same reactor configuration as considered by the chemist, while inventing the process. So, that point we note, for preliminary designs, use the same configuration as used by the chemist. Now, the kinetic data is also very important while deciding the size of the reactor, in most of the cases, you may not have kinetic data.

Therefore, we cannot evaluate at initial stage, the influence of reactor configuration on product distribution of course, this discrepancy can be removed, as we go further and further with flowsheet synthesis. So, that point we are noting, we cannot evaluate at initial stage the variation in product distribution with reactor configuration, designing detail designer reactor is quite effort intensive.

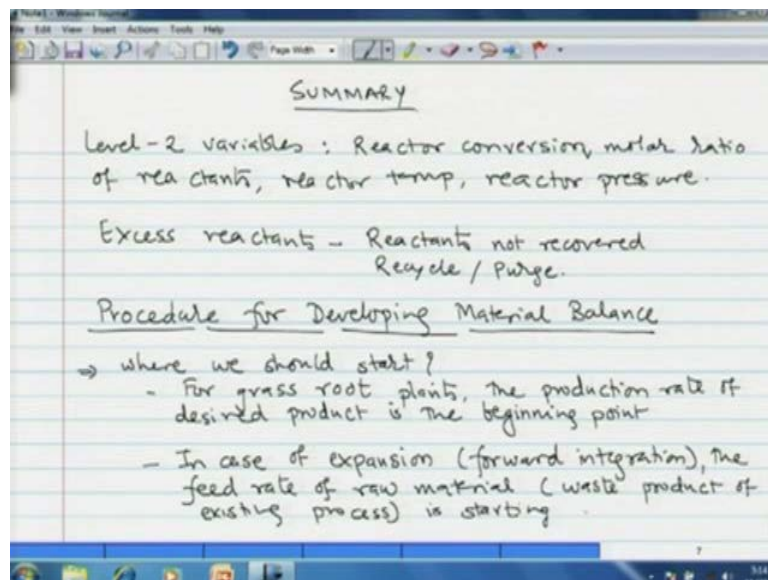
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So, the preliminary calculations should justify additional effort taken for designing of the reactor. Now in addition, what are other variables, that enter into the material balance is 1st is, whether we are going to recover and recycle all reactants and 2nd as I said at the beginning of the lecture, the use of gas recycle and purge stream. Now, when we talk of recovery and recycling of reactant then the percentage recovery is an important variable then when we talk of using a gas recycle and purge stream, the first thing that we have to specify is, how much excess gaseous reactant, that will be fed to the process.

Now, this excess will most of the time define in terms of molar ratio to the limiting reactant and this decides the amount of unreacted gas, that will come out along with the innards. And then we have to decide, as what fraction of this unreacted gas will form the recycle stream and the remaining purge stream. So, the composition of the gas recycle and purge stream is another variable, that comes in the picture so that point we note, molar ratio of reactants. Then next is the excess reactant, that is fed to the system, then next is the amount of innards that form, the innards that enter with the feed stream and the innards are forming the process. And finally, the ratio of recycle to purge, as what fraction of unreacted gas is recycled and how much is thrown out, and this decide the molar composition of the recycle purge stream.

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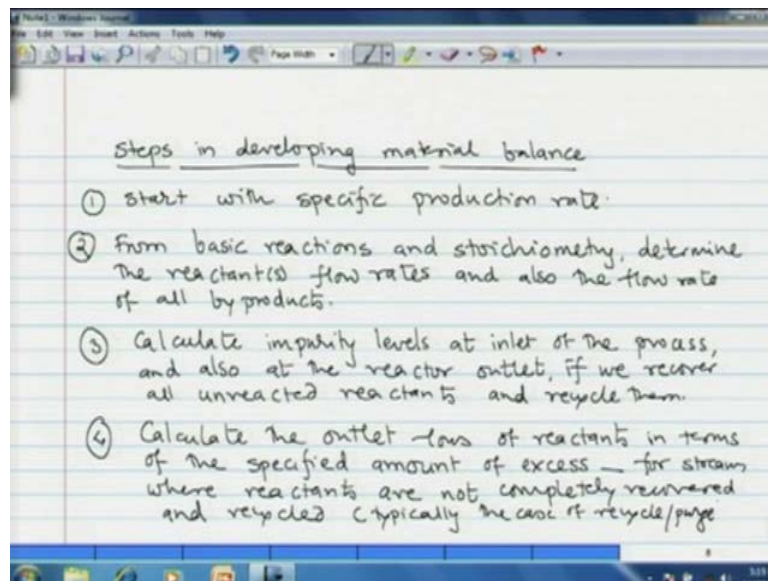
So, now we summarize the design variables, level 2 variables, reactor conversion, molar ratio of reactants then the reactor temperature and pressure. I am not including here

reactor configuration because as I just said in the preliminary level, these details are not included. The economic potential at preliminary level should be sufficiently promising to take up this additional effort and for excess reactants, reactants not recovered and the recycle purge stream.

Now with this, we shall see the procedure for developing overall material balance, the first question that comes is that, where we should start our calculations. In case of grass root plants, which are built from scratch, the production rate of the product decides or is the beginning point or starting point for the material balance calculations. However, in some cases, the company may would like to do forward integration which means, the company may want to set up an additional unit, that uses one of the waste products of the existing process as input and it is converted to a value added product.

Now, in such cases, the starting point of material balance is the feed rate so that point we note, where we should start. For grass root plants or completely new plants, the production rate of desired product is the beginning point. In case of expansion or what is also known as forward integration of the process, the feed rate of raw material, which is the waste product of existing process or byproduct of existing process is the starting point.

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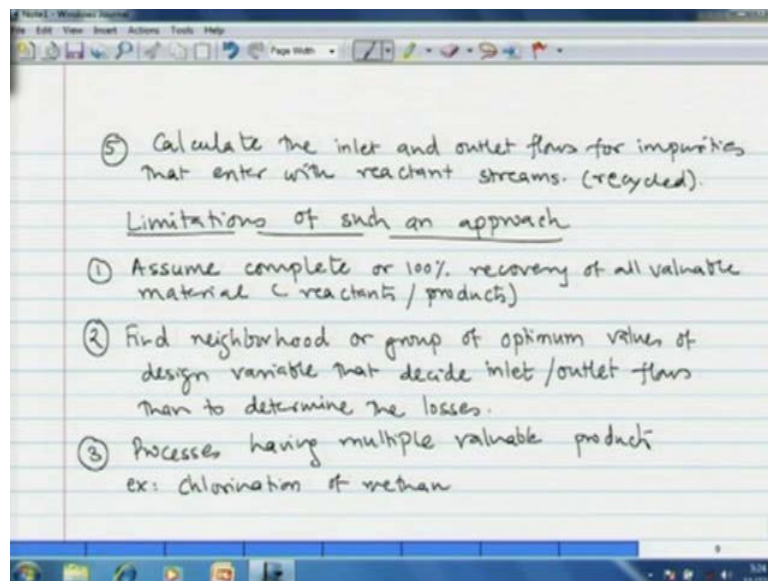


Now, let us see the first case, which is an easier version, steps in developing material balance, step 1 start with specific production rate, next from basic reactions of the

process and stoichiometry, determine the reactant requirement or reactant flow rate and also the flow rate of all byproducts. Now, while deciding the reactant flow rate, the per pass conversion of reactor is a variable of course, we shall see that later. The selectivity of the process is also a variable therefore, the material balances are most of the times iterative balances. Because, one parameter depends on another, another depends on third and then you come back to the first parameter so on and so forth, but right now, we are listing only the major steps.

Next is, calculate the impurity inputs or impurity levels at the inlet of the process and also at the reactor outlet, if we recover all reactants and recycle them. As I mentioned previously in this lecture, some impurities may enter with the feed stream and some byproducts or innards may also form within the process. Next is, calculate the outlet flows of reactants in terms of the specified amount of excess now, this is particularly the case for streams where, the reactants are not completely recovered and recycled, this is typically the case, when a gas recycle purge stream is used.

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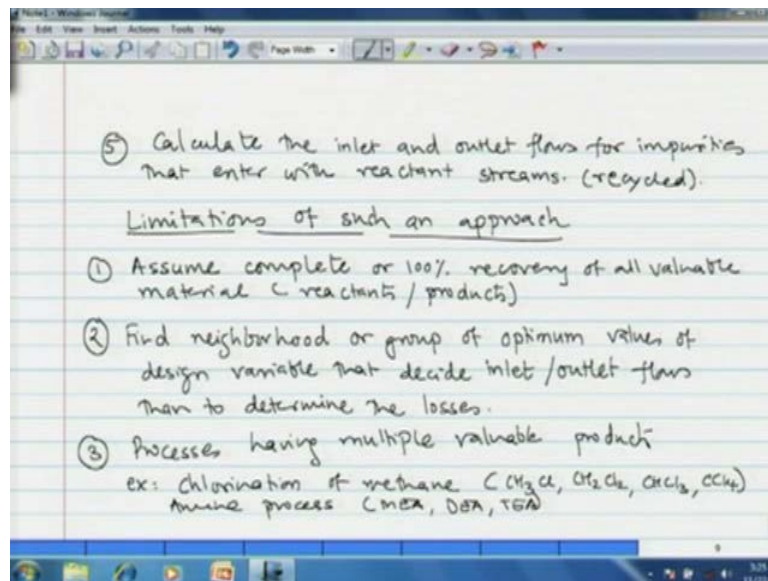


And finally, last step is to calculate the inlet and outlet flows for impurities, that enter with the reactant stream basically, the recycle reactants, which we calculate in step 4. Now, this is a very general approach for material balance calculations, which could be applicable to any process. However, this material balance has certain limitations because it makes certain assumptions.

So, let us also identify the limitations, limitations of such an approach, now the 1st limitation is that, we assume 100 percent recovery of all valuable material, which may not be possible. I am using word material because it includes both reactants and products and byproducts now, it is always more important to find the neighborhood of optimum values of design variable, which fix the inlet and outlet flows than is to include the losses early in the analysis.

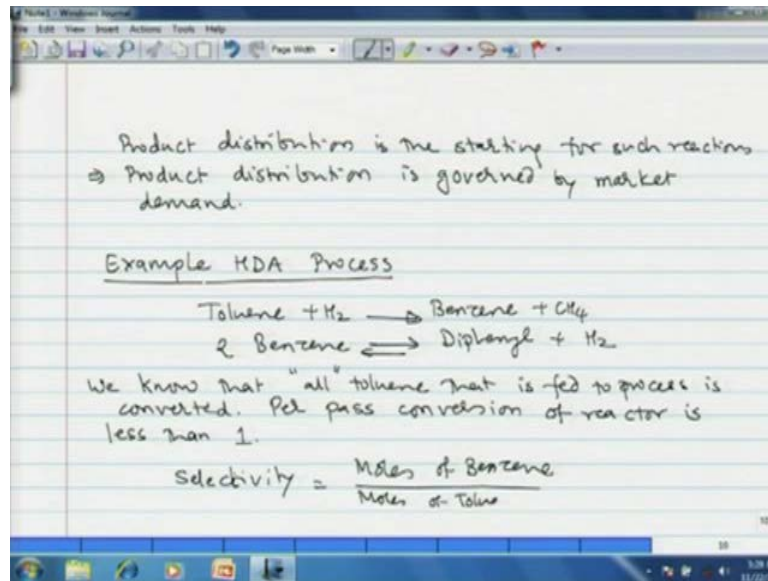
So, that point we also note, that find the neighborhood or a group of optimum values of design variables, that decide the inlet and outlet flows than to determine the losses, as we have seen in step 4 and step 5 of our approach. Now, the approach that we have seen essentially, focuses on predominant production of a single product and along with some unwanted side products. But in many processes, there are several valuable products, the example is like chlorination of methane where, successive substitution of hydrogen atoms in methane by chlorine molecule gives a rise to 4 products.

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Methylene chloride, methyl chloride then methylene chloride, chloroform and carbon tetra chloride, all of these 4 products are valuable. Now in such cases, we have to decide first the product distribution and then start the material balance. Another example could be that of amine processes where, monoethylene amine, diethylene amine and triethylene amine are the products and then again you have to first go for the product distribution and then start the material balance.

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That point we note here, product distribution is the starting point for such reactions, which have multiple products and product distribution in turn is governed by the market demand obviously. Now, we shall see the example of the HDA process, as how we can develop a material balance, which is in terms of design variables. I briefly give the basic chemistry again HDA process, toluene reacts with hydrogen irreversibly to give benzene and methane, and 2 molecules of benzene combined reversibly to give diphenyl plus hydrogen.

Now we know, that all toluene that if fed to the process is converted but all toluene essentially means, the fresh toluene. Because, the per pass conversion of the reactor could be less than 1, is always less than 1, in fact. So, this would leave large amount of unreacted toluene at the reactor outlet, and which has to be recovered and recycled. Now, we define selectivity for this process now, general definition of selectivity has already been given in the first lecture of this module.

There are 2 ways of defining selectivity, either the moles of desired product formed divided by the total moles of limiting reactant converted or the moles of desired product formed divided by moles of undesired product form so we use the forward definition. That is, moles of benzene formed, which is the desired product of the process divided by moles of toluene that are converted.

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Assume that we recover and remove all benzene.

Desired production rate of benzene: $P_B \frac{\text{mole}}{\text{h}}$

Feed rate fresh toluene $F_{FT} = \frac{P_B}{S}$

Production rate of methane in reaction $P_{R, CH_4} = \frac{P_B}{S}$

Fraction $(1-S)$ is lost to diphenyl however, stoichiometry of 2:

Production rate of diphenyl: $F_{FT} \left(\frac{1-S}{2} \right) = \frac{P_B \times (1-S)}{2S}$

Toluene contains no impurity.

We also assume that, we recover and remove all benzene now, as I just mentioned at steady state of the process, all of the fresh toluene should get converted, otherwise there will be an accumulation of toluene in the flow rate. Now, let us say, that the desired production of benzene, desired production rate of benzene is P_B mole per hour then obviously, the feed rate of fresh toluene, which we denote by letter F_{FT} is $\frac{P_B}{S}$, the selectivity.

Now, if you go to the basic reactions stoichiometry then you would find that the production rate of methane in reaction, which we denote as P_{R, CH_4} is also $\frac{P_B}{S}$. If fraction S of toluene is converted to benzene, the fraction $1 - S$ is lost to diphenyl however, since the stoichiometry is 2, which 2 molecules of benzene gets converted to 1 molecule of diphenyl. We write the production rate of diphenyl as $F_{FT} \times \frac{1 - S}{2}$ or $\frac{P_B \times (1 - S)}{2S}$. Now here, we have assumed, that toluene contains no impurity and there are no additional side products.

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Recycle and purge:

H₂ balance of the process:
$$\left[\text{H}_2 \text{ fed to process} \right] = \left[\text{H}_2 \text{ utilized in reaction} \right] + \left[\text{H}_2 \text{ generated in process} \right] + \left[\text{Excess H}_2 \right]$$

$$Y_{FH} F_G = \frac{P_B}{S} + \frac{P_B}{S} \frac{1-S}{2} = F_E$$

Methane balance: Total Prodⁿ of Methane $P_{CH_4} = \underbrace{(1-Y_{FH}) F_G}_{\text{Methane entering through fresh gas}} + \frac{P_B}{S}$ } Purge methane

(P_G)
Purge Stream (total) = Excess H₂ + P_{CH₄} = $F_E + (1-Y_{FH}) F_G + \frac{P_B}{S}$

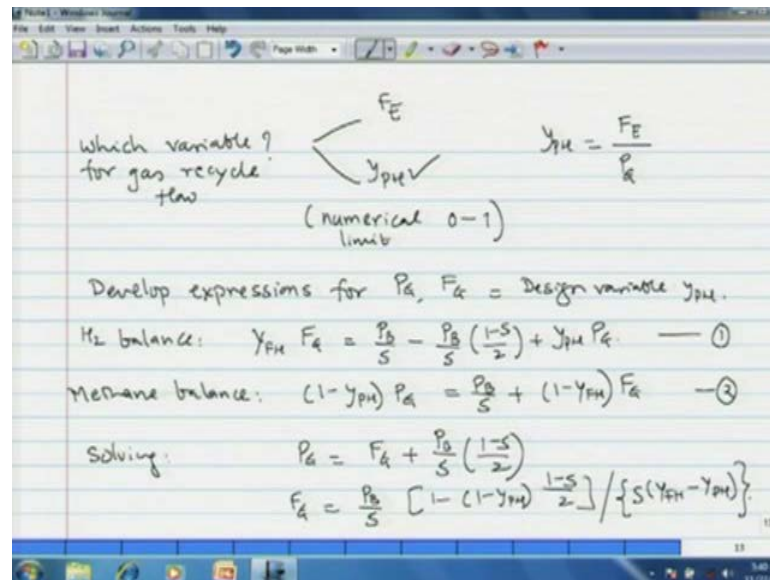
Now, let us focus on the recycle and purge stream, let us now do the hydrogen balance of the process, we are feeding an excess of hydrogen to force complete conversion of toluene. So, the hydrogen fed to the process is equal to, the total hydrogen that is fed to the process is hydrogen utilized in the reaction, the first reaction. And then the hydrogen that is generated in the process we saw that, when 2 molecules of benzene combine to give diphenyl, hydrogen is generated in the process plus the excess hydrogen, that is left as unreacted so this is basic balance on hydrogen.

Now, if we say that, Y F H is the mole fraction of hydrogen in the fresh gas stream, which we denote as F G then the fraction of this hydrogen that is utilized in the process is P B by S, by stoichiometry. And the hydrogen that is generated in the process is seen as the production rate of diphenyl, which is P B by S into 1 minus S by 2, as we just derived and that should be the excess hydrogen, that is left at the reactor outlet.

Now similarly, we do the methane balance now, as I just said that, we have to ensure that at steady state of the process, all the innards that enter in fresh feed streams and all the innards that generate it in the process should be purged, otherwise there will be net accumulation of these innards into the process. Now with this guideline, we can write the total production of methane, that we denote as P C H 4 is equal to 1 minus Y F H into F G, which is the methane entering through fresh gas stream and then the methane that is generated in the process P B by S. Now, this is the purge methane, the methane that is in

the purge stream however, the purge stream total should comprise of excess hydrogen plus methane, that is produced in the process. And therefore, the expression for the purge stream is F_E plus $1 - Y_{PH}$ into F_G plus P_B by S , the purge stream we denote by letter P_G .

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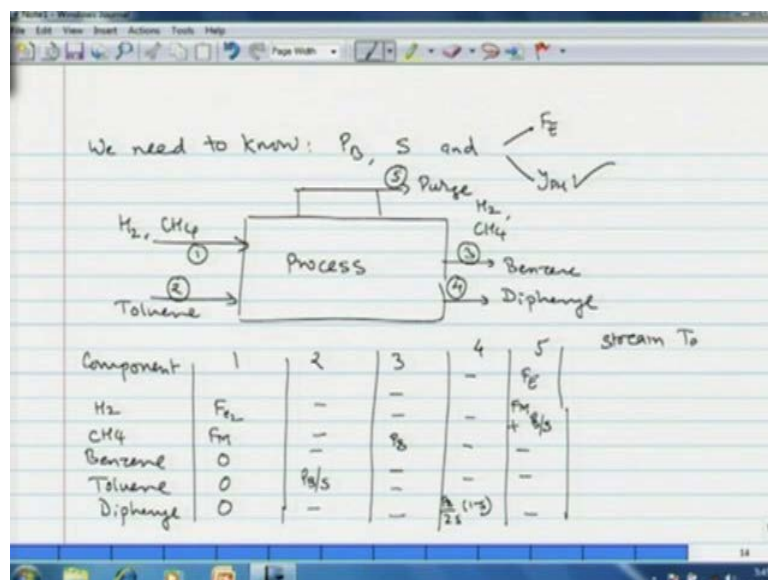
Now, which variable we should use, we had 2 options for deciding the gas recycle flow, either the excess hydrogen that is fed to the process or the composition of hydrogen in the purge stream, that we denote as Y_{PH} . Y_{PH} essentially is the excess hydrogen, that is fed to the process divided by the total purge flow now out of these two, we prefer to use Y_{PH} as the variable, because of numerical advantage. Y_{PH} is essentially a mole fraction of hydrogen in purge gas and being a mole fraction, it has numerical limit of 0 and 1, mole fraction has to fall between 0 and 1. So, it helps in solving material balance, if you use Y_{PH} as the design variable.

Now, we try to develop expressions for P_G , purge gas and F_G , and this will be in terms of and the design variable Y_{PH} . Now, once again we write the hydrogen balance, the hydrogen that comes in with fresh gas Y_{PH} into F_G is either utilized in the process plus the hydrogen that is generated into the process. But, we are now writing it on the right hand side, it is negative plus the hydrogen that is purged. Now, all hydrogen and methane, all excess hydrogen and methane should leave in the purge stream therefore, methane balance can be written as the methane that is purged is $1 - Y_{PH}$ into P_G .

Y P H is the mole fraction of hydrogen so 1 minus Y P H is methane, fraction in the purge gas and that should be equal to the hydrogen generated into the process P B by S plus the hydrogen, that has entered the process with fresh gas.

Now, we have essentially 2 equations with 2 unknowns, F G and P G, and now if we solve them, if we just add the 2 expressions then we get, this thing P G equal to F G plus P B by S into 1 minus S by 2. And then if we solve for F G then we get P B by S into 1 minus Y P H into 1 minus S by 2, divided by S into Y F H minus Y P H. Now, we can see that, in this entire material balance that we have developed, we need to know only few variables to calculate all the stream values.

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What we need to know, if we know P B production rate of benzene, which is the basic factor beginning point of this material balance, if we know the selectivity and either F E excess hydrogen or Y P H, we can calculate the flow rates of all streams. Now, as I just mentioned, because of numerical advantage, we go for Y P H thus now, we can write a stream table.

First we draw the process then we number the streams like the two feed flows or numbered as 1 and 2 then we number the purge stream as methane and hydrogen. Then benzene and diphenyl, will give number 3 to benzene steam which is the primary product, 4 to diphenyl which is the secondary product, side product and number 5 to the

purge stream. Of course, we also have a recycle stream but that we are going to see in the next chapter that is, the recycle structure of flowsheet.

And then we can make a stream table, we list all the components H_2 , CH_4 , benzene, toluene and diphenyl and then in each stream, we try to identify the exact composition. For example, in the first field stream, the hydrogen is F_{H_2} and F_{H_2} is essentially the excess hydrogen plus the sum of hydrogen that is produced and utilized in the process, that I am giving expression directly but it is very easy to derive it then methane is F_M but F_M is essentially $1 - Y_{FH}$ into F_G .

Now for F_G , you can put the previous expression and get a complete expression, there are no streams associated with it. The second stream, which is toluene contains only toluene and the flow rate is P_B by S , as we just derived, the number 3 stream, which is primary product contains only benzene, that has production rate of P_B and no other product.

Then number 4 stream, which is diphenyl contains diphenyl, which is P_B divided by $2S$ into $1 - S$ and no other component. And number 5 stream contains hydrogen, which is excess hydrogen and the methane, the methane that comes with the fresh stream plus the methane, that is generated in the process and no other component so we have essentially prepared a stream table.

In the next lecture, we shall see an alternate approach to material balance in terms of reaction coefficients where, we can write the entire material balance of the process in matrix form, which is easier to solve on a computer. In addition, we shall see, as how we can use these stream table to evaluate the economic potential of the process. Having done the overall material balance of the process, we have the information of the product values, the byproduct values and the cost of raw materials. And also, the alternate routes to the byproducts for example, diphenyl produced in the HDA can be used as a fuel, the purge gas that comes from HDA process can also be used as fuel. So, we shall see, as how these side products values add to the economic potential so the next lecture would be on determination of economic potential of the process.