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Module - 2 Flowsheet Synthesis (Conceptual Design of a Chemical Process) Lecture - 8 Recycle Structure of Flowsheet (Part II)

Welcome, we are looking at a Recycle Structure of the Flowsheet. In previous lecture we saw the basic decisions that we need to make while fixing the recycle structure of flow sheets. And then we also dealt with appear of the decisions, such as the number of reactor systems, the number of recycles dream, use of excess reactant.

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Today, we shall see the material balance with recycles streams, we have already seen the material balance for the overall process in the form of input output structure of flowsheets. We now open that process box, that we drew in case of input output structure of flowsheet, and make it into 2 boxes, first is the reactor system and then separation system, and then we try to do material balance across these 2 boxes.

Let us start with the HDA process, hydrodealkylation process as example, here toluene is reacted with hydrogen to give benzene and methane, and 2 moles of benzene undergoes reversible reaction to produce diphenyl hydrogen. Let us try to draw a simple recycle structure of the process, as a set that we now open the process box and split it into reactor and separation system.

We have not specified what kind of separation system we are going to use but we know that, from separation system 2 streams will emerge, one is the liquid stream and second is the recycle and purge stream. We have already said decisions, under which have to use recycle and purge system, though the 2 feeds streams to the reactor, hydrogen with impurity of methane and toluene. And the reactor effluent goes to the separation system, which splits the effluent into 2 parts, the liquid phase and gas phase.

The gas phase stream coming out of this operation system essentially is unreacted hydrogen with methane and liquid recycle stream is unconverted toluene. Let F T denote the total toluene feed to the reactor, out of which some parts comes as a recycle streams and other as fresh stream. So, the fresh toluene that is fed to the reactor is denoted by F F T and now, we try to do material balance for a certain production rate of benzene and also diphenyl as a side product.

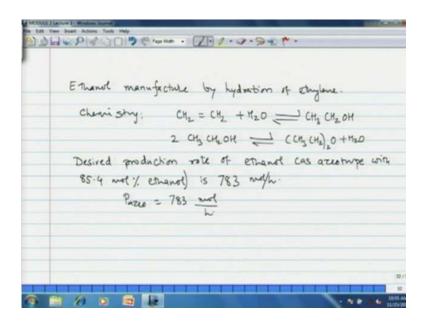
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If you do the material balance at the reactor inlet, the total feed of toluene comes from the fresh toluene and the unconverted part of total toluene feed. Now, let us say, that x is the per pass conversion in the reactor and therefore, the toluene that comes out and reacted is F T into 1 minus x. We assume that all of this toluene is recovered in the separation system and recycle back to the reactor. Now, if you simplify this particular expression then we get, a relation between fresh feed of toluene and total feed of toluene.

The total feed of toluene is F F T by x now, this material balance is always valid in case of, limiting reactant, however we have to assume complete recovery and recycle of limiting reactant. Now in some cases, the limiting reactant may leave with the product or in the purge stream and therefore, we have to slightly modify the balance. But, we will see now, again with an example that, the general relation between the total feed of limiting reactant and the fresh feed remains same.

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We now see, example of ethanol manufacture by hydration of ethylene, the basic process is ethylene reacts with water reversibly to give ethanol and 2 moles of ethanol, again combine reversibly to give diethyl ether and water. Let us say that, a desire production rate of ethanol as isotrope with 85.4 mole percent of ethanol is 783 mole per hour. Remember, that ethanol is being produced as a isotrope with 85.4 percent of ethanol now, let us now try to draw the recycle structure of this particular process.

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Hat	, <u>сн</u> 4	NERCION	Seperation .	-> Etok. 40 azotnyc.		
		DEE	H20	Limiting reactant is water.		
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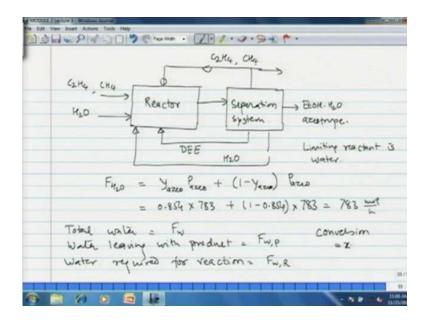
The process will comprise of single reactor, because both reactions have same temperature pressure conditions. Then there will be a separations system comprising of displacing columns, which will give ethanol isotrope as product then there will be a recycle and purge stream for unreacted ethylene. The ethylene may also have some impurity of methane and the 2 side products diethyl ether and waters are recycle back to the reactor. Here, the limiting reactant is water and some water leaves the process with isotrope now, we try to give the balance in a similar way, as we did for HDA process.

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POPErune . Z. 1. J. S. P. Ethanol manufactule by hydration of ethylane. chemistry: CH2 = CH2 + M20 = CH2 CH2 OH 2 CH3 CH2 OH = (CH3 (H2) 0 + H20 Desired production rate of ethand cas accorrupe with 85.4 mot 1/ ethanol) is 783 moth Pazzo = 783 mol $\frac{1}{2}$ $\frac{1}$

So, the production rate of isotrope Pazeo is 783 moles per hour, this contains absolute ethanol 669 mole per hour like, Yazeo is the mole faction of pure ethanol or absolute ethanol in the isotrope. Then the amount of water that is in the product stream is 783 minus 669, which is 114 mole per hour.

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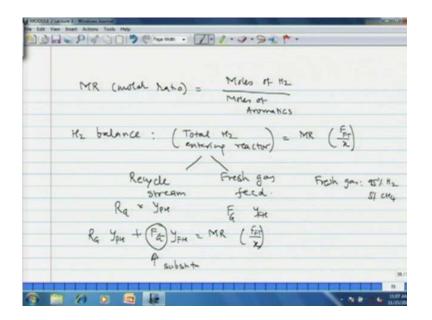
Now, the water that is fed to the process, which we have to write in the recycle stream should comprise of the water, that is leaving with the isotrope and also the water that is required for the reactions. So, the water stoichiometry is 1 so the water that is required for reaction is same as the production rate of absolute ethanol and the water that leaves with the as isotrope is 1 minus Yazeo into Pazeo. So, if we substitute values 0.854 into 783 plus 1 minus 0.854 into 783, we get 783 mole per hour so the total feed of water to the reactor system should be 783 mole per hour. Now we say, that a total amount of water that is entering is F W, the water that is leaving with the product is F W P, water required for reactions is f w r and the conversion is x.

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	Bolance for water
	$(F_{w,p} + F_{w,R}) + [F_{w}(I-X) - F_{w,p}] = F_{w}$
	Flow of other components
-	O Flow rate of limiting reachant
	() Molar ratio

Balance for water is F W P plus F W R plus F W into 1 minus x, minus F W P is equal to F W and then if you simplify this, we get a very similar expression as in case of a HDA process. F W is F W R by x, the total feed rate of water is the water required for reaction divided by the conversion. We have to complete the material balance to calculate flow of other components of the process, now we know at this stage, is the flow rate of limiting reactant, both fresh reactant as well as recycled. And then we have to specified the molar ratio of other components to the limiting component now again, we go back to HDA process as example.

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Here, the other component of other reactant is hydrogen and it is feed in excess so let us say, that M R denotes molar ratio, the moles of hydrogen to the moles of aromatics. Now, I am using here word aromatics instead of toluene because we may also consider in the later discussion, recycling of diphenyl to the reactor system. So, the total aromatics is toluene plus diphenyl in case diphenyl is recycled or only toluene, if diphenyl is taken out as a side product.

Now, if we see the hydrogen balance for the process, the total hydrogen that enters the process is molar ratio into F F T by x, which is the moles of aromatics or toluene and then these hydrogen should come from recycle streams and fresh gas feed. Now, let the total flow rate of recycle streams be R G and the mole faction of hydrogen in that stream be Y P H.

Now, we have used to Y P H as a notation for the mole fraction of hydrogen in purge gas however, we should see that, the purge gas and recycle gas are originated from the same separation. So, the composition is same, it is the same stream that is coming out of reactor separation system, that is split in 2 parts. So, the mole fraction of hydrogen in both the stream is same and therefore, we can use Y P H as the variable in calculating the hydrogen balance.

Let us say, the fresh gas feed rates is F G, the total molar low and Y F H be mole fraction of hydrogen in the fresh gas. Now, we have specified earlier, that the fresh gas comprises of 95 percent hydrogen and impurity of 5 percent methane. Now, Y P H is a variable, how does is affect the material balance, that we are going to see in detail in the tutorial following the lectures, right now we use letters variable.

Therefore, the balance is R G into Y P H plus F G into Y F H equal to M R into F F T by x. Now, when we did material balance for the input output structure, we had derived an expression for fresh gas feed rate and that, I would like to write again. It was F G is equal to P B by S divided by Y F H minus Y P H into, 1 minus Y P H into 1 minus S by 2. Now, the derivation of this equation was already discussed in the previous lecture, when we study input output structure, so I am now borrowing this expression directly.

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POP CONS - ZP - 9 $F_{\xi} = \frac{P_{B}}{s} \frac{1}{(\gamma_{Fu} - \gamma_{PH})} \left[1 - (1 - \gamma_{PH}) \frac{1 - \gamma_{PH}}{2} \right]$ $R_{q} = \frac{P_{B}}{S y_{PH}} \left(\frac{MR}{\chi} - \frac{y_{FH}}{y_{FH} - y_{PH}} \right)$ Design variables : PB, S. Joh, MR, X. Reversible reactions : Conversion - x equilibrium xey Good quess: X = 0.96 xeq.

If you substituted F G in the previous balance here and simplify then we get, an expression for R G in terms of the production rate of benzene, the selectivity, the mole fraction of hydrogen in purge stream and mole fraction of hydrogen in fresh stream. So now, we have all the material balance in terms of design variable P B, S, Y P H and M R now obviously, the optimization will depend on these variables, which we will see in the subsequent lectures.

In some cases, the reactions are reversible now for this reactions, the conversion x is a design variable of course, the design variable, which we list earlier also includes x, that we left out. So, the designed variables are 5 P B, S, Y P H, M R and x now, for reversible reaction, conversion x and equilibrium conversion x e q are the main variables. Now, how we should decide, as how much should be the conversion, there are no thumb rules available. However, a good guess would be that, x equal to 0.96 or may be 0.98 x e q, that we are approaching equilibrium conversion to maximum extend.

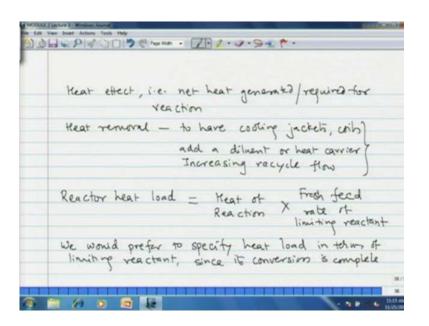
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Reve	sittle byproduct of HDA process
	2 Benzene _ Diphangel + H2
	$Kep = \frac{(Diphenyl)(H_2)}{(Benzene)^2}$
REAC	TOR HEAT EFFCT : Answering the guessim whet to operate reactor adiabatics or isothermally ?
	takon of temperature - exotularic

Now, in case of HDA process, the reversible byproduct is diphenyl, HDA process has 2 reactions, one is a irreversible reaction and second is a reversible. So, 2 moles of benzene giving diphenyl and hydrogen now, the extent of diphenyl in the reactor effluent will be decided by equilibrium constant and the relation would be this. Now, we will see in the tutorial, actual calculation of diphenyl using this so that completes the topic of the recycle material balance.

Now, let us see the reactor heat effects, one of the decision that we have to make is, whether to operate reactor isothermally or adiabatically and to answer that question, we need to look into the reactor heat effects. So, we note here, answering the question whether to operate reactor adiabatically or isothermally in many cases, there will be a limitation to the temperature achieved in the reactor, this is for exothermic process. For endothermic process, we have to supply heat however, to answer the question, whether we have to operate the reactor adiabatically or isothermally, we have to see the heat effect of the reactor.

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That is, the net heat generated or required for the reaction now, in case of heat removable from the reactor, we have several option like to have cooling jackets or cooling coils or in some cases, we add a diluent or heat carrier or we also add, we increase a recycle flow so on and so forth. However, to choose between these options, we need to first know the heat generated or the reactor heat load, whether positive or negative, is essentially heat of reaction multiplied by the fresh feed rate of limiting reactant.

We would always like to specify reactor heat load in terms of fresh feed rate of limiting reactant because conversion of fresh feed limiting reactant is complete. That point we note, we would prefer to specify heat load in terms of limiting reactant since conversion is complete. If we use these instead of, the fresh feed, total feed then we have to specify conversion, extent of conversion and there will be the large recycle flow fund so forth. So, it is much easier to do calculation in terms of fresh feed rate.

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Adiabatic temperature change of reactor - Th That reactor will achieve if all heat generated/required for reaction is supplied by the reactor contents HDA process: - 21,530 Btre not toluene Net heat liberated : -21,530 x Ps- beneene production rete S- selectivity (265 mol ~ 273 5 = 0.98 Sile = -21530 × 273 = -5,878 × 10

Now before we decide, how to remove or add heat, we have to see the adiabatic temperature change of the reactor. This means, that the temperature that the reactor will achieve, if all heat generated or required for the reaction, is supplied by the reactor contents or the disciplinary reactants. Again we take the HDA process as example, the heat of reaction of HDA process is minus 21530 B t u per mole toluene.

Therefore, the net heat liberated would be minus 21530 into P B by S where, P B is the production rate of benzene and S is selectivity and we have already derived this relation, fresh feed rate of toluene is P B by S. Now, we had considered example of production rate of benzene at 265 mole per hour and selectivity as, let us say, 0.98 or 96 so the F F T is approximately 273 mole per hour. And then the net heat liberated delta H R is minus 21530 into 273 that is, minus 5878 into 10 to power 6 B t u per hour. Now, before we go for further calculation, I would like to give some conversion, unit conversion.

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-5.878×10 : 1150 F Rea ctants enter Per pass conversion = 75%. Reactor effluent: X Bencene: 265 ml/h went: gi mol/4 x Diphenge: 4 mac/h 496 mol/L Ke up gas : here de gas (Ro) : 3371

1 B t u is 1055 joules and with this, you can convert the calculation into SI units, in tutorial, we shall see calculations mostly in SI units, this is just learning principles so I am using previous units. So, for production of 265 mole per hour of benzene, the heat that is required is minus 7.78 into 10 to power 6 B t u per hour. Now, the reactants enter at temperature of 1150 degrees Fahrenheit and if we operate the reactor adiabatically then all of this heat generated in the reaction is absorbed by the reactants or the product basically.

Now, if we do material balance, if we substitute let us say, P B equal to 265 mole per hour, F F T is 273 mole per hour. And if we assume per pass conversion to be 75 percent and the hydrogen in purge stream as, mole fraction of hydrogen in purge stream as 0.4 then the reactor effluent is benzene, 265 mole per hour, unreacted toluene 91 mole per hour, diphenyl will be about 4 mole per hour.

We have to give the make up gas F G as 496 mole per hour and the recycle gas R G would be 3371 mole per hour. Now, I am writing these figures directly but you can very easily calculate these figures by putting these numbers into the expression, that we have derived earlier. In the tutorial, we shall see a direct calculation of the entire material balance using a math card sheet and then you can see these figures calculation further. However, now what we do is that, extra fusing benzene we take toluene 273 mole per hour for calculation of the adiabatic temperature rise. That means, the heat that is

generated in the process 5.8 million B t u per hour is absorbed by total toluene then make up gas and recycle gas. We do not consider at this moment the products now, what will be the exit temperature, if the entry temperature is 1150.

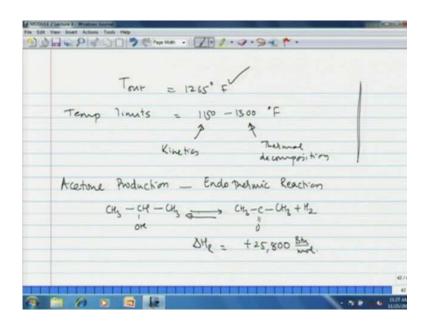
The unit of Q (beat transfer) is BTU/b as the mass flow rate, mis in mol/b. Keat balance ST = entry temp. -5-878 ×10 (273+91) 48.7 + 2º F CH. 10.1 (Tin - Trut) 48.7 3371×0.4×7 + 8371×0.6×10.1 3371 8.86 8m/mol .F

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Now for this, we have to do a very simple heat balance, Q is equal to M C P delta T where, delta T is T out minus T in, exit temperature minus entry temperature. Now, in order to calculate M C P, we need to know the molar flow rates, which have already listed and the molar heat capacities. The heat capacities of various components in B t u per mole per degrees Fahrenheit or hydrogen 7, methane 10.1 and toluene 48.7.

Now, with this we can quickly write the heat balance minus 5.878 into 10 to power 6 is equal to 273 plus 91 into 48.7 plus 496 into 7 plus 3371 into 8.86. Now, the 8.86 is the heat capacity of recycle gas, which we have calculated as molar flow rate of hydrogen, 3371 into 0.4 molar flow rate hydrogen into 7 plus 3371 into the methane fraction 10.1 divided by 3371, this transferred to be 8.86. Now, into is the M C P, see d T is T in minus T out now, we are writing reverse of delta T, that was written here because we have taken the heat as negative. If we take absolute heat then this becomes delta T as written T out minus T in.

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And now, we can very easily calculate the exit temperature as 1265 degrees Fahrenheit that means, if we operate the reactor adiabatically, the maximum temperature reached in the reactor is 1265 degree Fahrenheit. Now, in the previous lecture I had mention to you, the temperature limits for the HDA process, the temperature limits were 1150 to 1300 degrees Fahrenheit, the lower limit was fixed by kinetics and the upper limit was fixed by thermal decomposition.

And now we see that, even if all the heat that is liberated in the reaction is absorbed by the reactor contents, the temperature that is reached in the reactor is below the upper limit. Therefore, it would be easier to operate reactor adiabatically, we are not going to cross the limit, if we operate the reactor adiabatically; of course, we have not considered here the various loses that occur due to radiation, convection, so on and so forth.

In reality, the temperature that is reached will be lesser than 1265 degrees Fahrenheit so this is how, we decide whether to operate reactor adiabatically or isothermally. In some cases, you have to supply the heat of reaction, for example the acetone production now, this reactions is an endothermic reaction. The process is dehydrogenation of iso propenal and the heat of reaction here is plus 25800 B t u per mole. Now, these of course, is also reversible reaction, some reversible component is there now in this case, we have to supply the heat of reactions.

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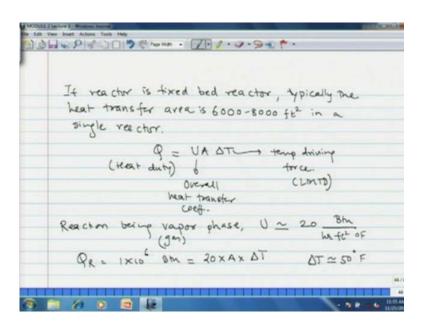
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Now, for a particular rate of production of acetone let us say, we take rate of production of acetone 51.3 mole per hour. The total heat required to be supplied to reactor is 51.3 into 25800 that is, 1.324 into 10 to power 6 B t u per hour. Now, let us say that, the entry temperature of reactant is 576 degrees Fahrenheit, now reactants mean both fresh as well as recycle.

If all the heat of reactions that is required is taken from the reactants, the temperature falls below 0 degree Fahrenheit, which is in practical and therefore, we have to operate reactor isothermally that is, we have to provide the heat of reactions. Now in this case, the reactor itself is a heat exchanger, in which the catalyst is packed in the tubes and ipa, the iso propenal again as an isotrope flows over the catalyst bed and then dowtherm liquid is condensed in the shell and the heat of reaction is supplied.

We shall see detailed calculations in an example, how does the reactor heat load influences the reactor design. If the reactions are catalytic reactions then we have options of having a fix bed reactor, a moving bed reactor, a fluidized bed reactor and in fluidized bed, there are mode of operation like bubbling fluidized bed or a circulating fluidized bed. However, the amount of reactant that can be processed in the single reactor is limited by the heat of reaction.

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Now typically, as a thumb rule, if the reactor is a fix bed reactor in the form of heat exchangers and as I just said that, the catalyst is packed in the tube, over which the reactant flows. Then typically, the heat transfer area that can be accommodate in the heat exchanger is about 6000 to 8000 feet square otherwise, the reactor size becomes excessively large.

Now, we know the basic relation in heat transfer Q is equal U A delta T, Q is the heat duty of the reactor, U is the overall heat transfer coefficient, delta T is the temperature driving force. We most of the time calculate it in terms of LMTD and A is the area of the reactor now, if the reaction is a vapor phase reaction, the overall heat transfer coefficients that can be achieved are limited. For example, for vapor or let us say, gas phase reaction, the typical U that can be achieved is about 20 B t u per hour per feet square per degrees Fahrenheit.

Now, if the heat load is 1 million B t u then the area that is required will be 20 into A into delta T. Now, let us assume that, we have a sufficiently high delta T of about 50 degrees Fahrenheit, this would be the case when we have, as I just said a condensing vapor in the shell and gas flow or vapor flow in the tubes, this is typically delta T, that we are likely to achieve.

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Area (per million Btr) = 1×10⁶ = 1000 ft² of heat long) = 20450 Total heat duty in a reactor ~ 6-8×18 8th This helps in determining motor flow rate of limiting reactor. HOA process = -5.8 ×10 Bh = Single Heat Carriers : Contact of King & Heat load fixed by freh feed note of Inviting reactant

Then, the area that is required, area per million B t u of heat load will be 1 into 10 to power 6 divide by 20 into 50 that is, 1000 feet square. Now, we have the limit of heat exchanger area in a single unit that is, 6000 to 8000 feet square. So this means, that the total heat duty in a reactor can be about 6 to 8 million B t u and on this basis, we can decide the molar flow rate of the limiting reactants.

For example, we just saw the HDA calculation where, the heat load was minus 5.8 into million B t u into 10 to power 6 B t u and this particular process could be carried out in a single reactor. We do not have to split the streams, if the heat load for a particular productions rate is higher than this then we will have to have 2 parallel reactors, in which the feed will be split in 2 parts. Let us see, the heat carriers or how do we control the temperature in a particular reactor, we just saw, that the reactor heat load is fixed by fresh feed rate of limiting reactants. Now, if the other reactants is fed in excess then we have a very large amount of unreacted reactant at the reactor outlet.

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Control of temp can be achieved by reguling of unreacted reactant or by product
a) Addition of extraneous component
HDA process: Methane (10.) Bty
Oxidation system: Nitrogen in air acts as heat arriched air diluent.

Now, to control the temperature, one easy way would be to recover and recycle of the unreacted reactant, control of temperature can be achieved by recycling of unreacted reactant, which acts as a heat diluents. It adds to the mass of the reactors and then tries to absorb the heat and control temperature or you can also recycle some of the byproducts, if they are not going to trigger any side reaction or you can also add an extraneous component like some inert like nitrogen or methane.

However, the cost of this extraneous component and then it is now, processing drive add to the overall operating cost. For example, in HDA process, we have the side product of methane, we just a saw that methane has sufficiently high heat capacity of 10 B t u per mole per degrees Fahrenheit. If you recycle more gas, more unreacted hydrogen along with methane, the methane acts as a heat diluents.

We saw that, methane was not triggering any side reaction in the process but because of it is high heat capacity, relatively high heat capacity, it can help in controlling the temperature of the process. Same thing happens in case of oxidation system here, nitrogen in air acts as heat diluents now, in order to reduce the cost of compressor, one of the options process alternative that is used in HDA process is, purification of the recycle gas that is, taking out hydrogen and throwing of methane.

In some cases, in case of oxidation system, enriched air is used where, the oxygen content of air raised from 20 percent, which is normal to 40, 50 percent. Now, this

reduces the load on compressor however, we also need to see the other side of coin that, less content of methane in recycle gas, in case of HDA process or less content of nitrogen in air can give arise to surge of temperature.

And therefore, in that case, we will have to take additional precautions to remove the excess heat so that, the temperature limit is not crossed, if recycle gas then of course, the compression cost desire but at the same time, we do not have to worry about the temperature surging. In the next lecture, we shall see the actual reactor design or reactor design protocol and we shall also see some examples.