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Module - 2 Flow Sheet Synthesis (Conceptual Design of a Chemical Process) Lecture - 11 Tutorial (Part II)

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Welcome, we are now approaching the end of module 2 that is flow sheet synthesis. So, far we have seen various aspects of flow sheet synthesis, various levels of flow sheet synthesis, the decisions that we have to make at each stage. Thereafter, we also dealt with a few problems on the selectivity in a parallel reactions as well as series reactions. Now, in this lecture, which is the second tutorial of this module, we shall deal with the selectivity in multiple reactions which are neither necessarily parallel or series.

We shall also see some problems on synthesizing of flow sheet and determination of the economic potential of the flow sheet at various stages. So, we start with the first problem; that is the selectivity determination in multiple reactions. Now, let us see the problem statement first. Consider the reactions, A plus B goes to C with rate constant k 1 and A plus C goes to D with rate constant k 2. Now, C is the desired product and D is the

underside or waste product. Now, these reactions are carried out in CSTR at 10 degree centigrade and 6 bar pressure.

The flow rate of the reactant A and B is q, unit may be meter cube per second and the volume of the reactor is V meter cube. Now, we have to determine the selectivity in terms of conversion of the limiting reactant A. Determine the selectivity in terms of conversion of limiting reactant A. Molar ratio of the reactants the initial molar ratio at the point of entry, you can take as V naught by A naught and this molar ratio is indicted by letter M.

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The time constant or the residence time of the reactants will be equal to the volume of the reactor dived by the volumetric flow rate. We already know that molar ratio is B naught by A naught and now what we do is that we denote the moles of the four component of the system by the same letter A, B, C and D. Now, at any time T greater than 0, the net change of moles of A which is A naught minus A would be equal to tau into k 1, the rate constant into A and B and plus k 2 into A into C.

Similarly, B naught minus B, the change of number of moles of B would be equal to tau into k 1 into A into B. The number of moles of the two products formed C and D will be, for C it will be tau into k 1 into A into B minus k 2 A into C and for d it will be, tau into k 2 into A into C. The selectivity S will be equal to C the desired product divide by the limiting product converted, A naught minus A.

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$\frac{c}{8-8} = \frac{\kappa_1 A B - \kappa_2 A C}{k A B} = \frac{1-\kappa_1 C}{8}$	
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Making an above exercise explicit in C	
B-B7	
$C [1+K] = B_0-B$	
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1+K (80-3)	
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We can also write: C = (Bo-B) - (Ao-A)	
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We substitute for C as well as changes in the other excess component B C divide by B naught minus B. Then we get for C we substitute the expression that we just wrote k 1 into A into B minus k 2 into A into C divide by k 1 A. Thus we get the expression 1 minus capital K into C by B where capital K is the ratio of the rate constants of the two reactions. We make this expression explicit in terms of C.

You can simply rearrange the equation which is rather straight forward C into 1 plus capital K into B naught minus B by B divided is equal to B naught minus B under C is equal to B naught minus B divided by 1 plus K into B naught minus B by B. So, this is our first result. We can also write that number of moles of C formed or the number of moles of B reacted minus the number of moles of a reacted, based on material balance.

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Then we get A naught minus A is equal to B naught minus B minus C and now for C we substitute the expression that we just derived; A naught minus A is equal to... Now, B naught minus B is the number of moles of B converted, so we can write that in terms of the conversion of B x B is the conversion of B. B naught into x B minus for C we write the expression that we just derived. B naught into x B divided by 1 plus K into x B divided by 1 minus x B. Now, what I have done here is that I have converted the expression for C, in terms of conversion for B.

Now, that is rather straight forward that I show now x B is equal to B naught minus B divided by B naught. Therefore, B is equal to B naught into 1 minus x B. Therefore, C is B naught into x B divide by 1 plus K into x B divide by 1 minus x B. So, this is the essentially the transformed from of what we wrote earlier; that C was equal to B naught minus B divide by 1 plus K into B naught minus B divide by 1 plus K into B naught minus B divide by 1 plus K into B naught minus B divide by 1 plus K into B naught minus B divide by B naught. So, what we have done the previous expression, we have transformed into in the form of the conversion of B x B. Now, we go further with this the expression that we derived earlier.

A naught minus A was B naught into x B minus B naught into x B divided by 1 plus x into x B divided by 1 minus x B, that we now rearrange. A naught minus A is equal to B naught into x B into 1 plus k into x B divided by 1 minus x B minus 1 divided by 1 plus K into x B. This we can further simplify as B naught into x B divided by into K into x B divided by 1 minus x B whole divided by 1 plus K into x B divided by 1 minus A.

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A naught minus A, itself can be written in terms of conversion. Define x A the conversion of A, the limiting reactant as A naught minus A divided by A naught. So, A naught minus A is essentially A naught into x A and that we substitute in the previous expression. A naught x A, which is equal to A naught minus A is equal to B naught into x B into K into x B divided by 1 minus x B whole thing divide by 1 plus K into x B divided by 1 minus x B.

So, what we have now is; x A as function of x B, we further arrange this x A is equal to B naught by A naught by taking A naught here on the side into x B and we simplify. Now, this square bracket as K into x B divides by 1 minus x B plus x into x B. This becomes B naught by A naught is the molar ratio M. So, that we substitute M is into x B into K x B divided by 1 plus x B into K minus 1.

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Now, if you expand this, you get a quadratic in terms of x A in terms of x B which if you solve will give you an explicit expression for x B as function of x A. This I leave as exercise, it is simple I will give the final form of quadratic which you can solve M K into x B square is equal to x A into 1 plus x B into k minus 1. This is what you get, if you expand that the previous equation, which you can rearrange in the form of the our regular quadratic equation A x square plus B x plus C.

This is of from the... Then you know that the roots are minus B plus or minus B square minus 4 A C by 2 A. So, here you have A as M K. Now, A, B, C are not here do not confuse A, B, C with number of moles, but these are simple coefficients. So, A is M K, B is minus K minus K minus 1 and C is minus x A. So, if you simply substitute these three things in this equation the simple root, you will get the desired answer; that is x B as function of x A. Now this I have left as an excises, we back to the we can come back to the selectivity.

We have defined as the number of moles of desired product C formed divided by the number of moles of A, which is a limiting reactant converted. So, C divides by A naught minus A. Now, if we substitute the two things, we already have expression for C and A naught minus A in terms of x B. So, if you substitute that, substituting for C and A naught minus A in terms of x B, will give you the following.

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S =	$\frac{\beta_{o} \times \beta}{\left[1 + \frac{K \times 2\beta}{1 - \chi_{\beta}}\right]}$ $\frac{\beta_{o} \times \beta}{\left[1 + \frac{K \times 2\beta}{1 - \chi_{\beta}}\right]}$ $\frac{\xi_{o} \times \beta}{\left[1 + \frac{K \times 2\beta}{1 - \chi_{\beta}}\right]}$ $S = \frac{1 - \chi_{\beta}}{K \times \beta}$	$= \frac{1-\chi_{B}}{k\chi_{B}}$	
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S will be equal to C which we have obtained as V naught into x B divided by 1 plus K into x B divided by 1 minus x B. For A naught minus A we obtained B naught into x B and K into x B divided by 1 minus x B, whole thing divided by 1 plus K into x B divided by 1 minus x B. This can be simplified as 1 minus x B divided by K x B. So, we have selectivity in terms of the conversion of B. If you substitute for B x B in terms of x A by solving the quadratic equation that I gave earlier, you will get the desired answer.

So, that final answer I have left as an exercise for you. So, this is how you determine the selectivity in case of multiple reactions which are not necessarily parallel reactions or series reactions. So, we have dealt with all three types of selectivity's; we go to the next problem. In this problem we have to determine the economic potential of a particular process, but before that we have to do the material balance. Then we have to do some initial calculations, okay?

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So, let us try to do that first before we go to economic potential. The problem statement is on the screen, what we have is an energy integrated process for producing acetone from isopropanol, the flow sheet is on your screen. This is what is the flow sheet, you have the felid is the isopropanol azeotrope, I P H 2 O felid, which first go into a pre heater, then it goes into another exchanger that is Fe He felid to fluent heat exchanger, m then it goes to the reactor. Since it is endothermic process, you have to supply heat which is given by a furnace and the reactor effluent initially passes through the same feed we shall see the second problem of this tutorial.

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Problem 2: Flowsheet Synthesis for Acetone Process. CH3-CH-CH3 __ CH3-C-CH3 +H2 OR Feed : Accompe 70 met 1. Isopropanol. Heat of reaction : + 25,800 BM SI Heat Capacity of accompe: 22 3th 18m = 1.05 J of = 1.8 '6+32 Reactor conversion: 80 %. Inlet knows of me feed : 572°F Heat for reaction is supplied by conducing a Doutedu inp of contention = 610" in the reactor shell. The Gingil

That is the flow sheet synthesis for the acetone process. Acetone is manufacture by dehydration of isopropanol. We have the basic reaction as isopropanol getting decomposed to acetone and hydrogen. Now, let us see the basic aspects of this particular. The feed of the process is an azeotrope containing 70 mole percent of isopropanol. The reaction takes place in a CSTR where the heat is supplied for the reaction. Since, this is a decomposition reaction, it is an endothermic reaction.

The heat of reaction is plus 25,800 BTU per mole. The heat capacity of azeotrope is 22 BTU per mole per degree height the reactor conversion is 80 percent. The inlet temperature of the feed is 572 degrees Fahrenheit. Then you can easily convert these units into SI system by 1 BTU is 1.055 joules. You already know the conversion between degrees Fahrenheit and degrees centigrade, degrees Fahrenheit is 1.8 times degree centigrade plus 32, so this simple conversions, you can do.

The heat for the reaction is supplied by condensing the dowtherm liquid in the reactor shell. The reactor is essentially a shell and tube heat exchanger in which the tubes act with the catalyst. The reactant is opropanol flows in the form of vapor over the catalyst and the heat is supplied by condensing a dowtherm liquid vapors of dowtherm liquid into the shell of that particular heat exchanger. The temperature of condensation of the dowtherm liquid is 600 degree Fahrenheit

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Dowtherm liquid is reprised in a fulnace. Thermal efficiency fulnace = 60%. Heat losses in The pipe ~ 24% The final cost of the fulnace & 500 MM BTU Rocens operates for 8000 hours a year Queekons: () Draw I/p- 0/p structure of flowsheet (A) Detchnine me flow rates of all components at inlet and outlet of process. Drew regicle structure of flausheet: detchnine the recycle matrial balance Detchmine tuel cost annual

The dowtherm liquid is vaporized in a furnace, which is attached to the reactor and the thermal efficiency of this particular furnace is 60 percent. Then as the vapors of dowtherm pass transferred from the furnace to the reactor the heat looses in the pipes or the transport lines are above 20 percent. So, you can say the heat loss is about the, so the heat loss percent that is it the fuel cost of the furnace, which could be an oil fired furnace or diesel fire furnace can be taken as rupees 500 per m m BTU, million metric tons BTU and the process operates 8000 hours a year.

So, this is the data that we have for this particular process we have to answer following questions for the process, first draw the input output of the flow sheet, next determine the flow rates of all components at inlet and outlet of the process. Third is draw the recycle structure of flow sheet and determine the recycle material balance. Then the next is determine the annual cost of fuel for the furnace. Finally, determine the area for the reactor, I had told you that the reactor in the present case, is in the form of shell and tube heat exchanger. So, we have to determine the area of this heat exchanger.

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Let us start dealing with these questions one by one; the first question that is the input output structure of the flow sheet, since we have only one reaction in this particular process the structure is relatively simple. We have a process in which there is only one feed stream that is the isopropanol, water azeotrope and then there are three products; first is the main product acetone, then hydrogen and some water will come out. Now, how we shall see in few minutes, let us say we have not been given the production rate of acetone. So, we assume a simple rate production rate of acetone P A as 100 mole per hour. If you see the stoichiometry of the reaction, then the production rate of hydrogen will also be 100 mole per hour hmm the fresh IPA feed will also be 100 mole per hour.

I hope you recall that at steady state all the fresh reactant gets converted. So, if you see the stoichiometry 1 mole of acetone requires 1 mole of isopropanol, so the fresh isopropanol feed will be 100 mole per hour. So, all of these determine by stoichiometry, the feed is not pure isopropanol, but an azeotrope. So, the amount of water that enters with the feed will be 0.7 into 100 divided by W plus 100 where W is the total moles of the feed, so W becomes 42.9.

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Out of . Water	the ascotrupe,	isopwpa (42-3 c	not gets	converted	an
Flow reacto	to of the at	= 42-9	mit		

The total azeotrope will be 100 mole per hour of isopropanol plus the accompanying water, which is 42.9 mole per hour. So, total 142.9 mole per hour, so this is what will be at the inlet. So, we have determined all flow rates of all components at the inlet and out let of the, we summarize isopropyl, isopropanol, water azeotrope. 142.9 mole per hour acetone 100 mole per hour, H 2 O 100 mole per hour. Now, we have to we have not still yet determine the amount of water.

Now, that we shall do now out of this azeotrope, the isopropanol gets converted and water is left out that water will be 42.9 mole per hour. So, if we compare this particular process to the HDA process that we have seen. Water you can consider as an impurity

and then that has to be removed from the process at all time. Therefore, the flow rate of water at reactor outlet will be equal to 42.9 mole per hour.

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I/p- 0/p Structure	
PA = 100 met PA = 100 met	Acetone 100 mg Arocces Acetone 100 mg
Amount of 1600 in feed :	0.7 = 100 W = 42.9 200

Therefore, we write this parameter in the flow sheet H 2 O 42.9 mole per hour. Therefore, we have determine the complete input output structure of the flow sheet with the material balance. Let us see the recycle structure of the flow sheet.

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0.0	
	Total according = 100 ms IPA + 42.9 ml
	= 142.9 met
	Out of the azestupe, isoporpanel gets converted and water is left out (42 g and)
	Flow rate of the at = 42.9 mer / reactor onthet
	Recycle Structure : Pel pues conversion 80%.
	The ceparation system of process similar contain the distillation column, thist column remaining the main product aceture, and second column remaining
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The purpose conversion in the reactor is 80 percent. Therefore, there will be IPA unconverted, now that IPA will contain excess water, which is this 42.9 mole per hour

before recycling. We have to remove this water, so the outlet of the reactor the reactor effluent should pass through at least two distillation columns; in the first column the main product acetone will be removed from IPA and in the second column excess water will be removed from IPA.

So, in that column the main product will be IPA azeotrope, which will be recycled back at the reactor inlet reactant. It will be mixed with the fresh azeotrope feed, so that point we note that the separation system of the process should contain two distillation columns; first column removing the main product acetone and second column removing excess water from IPA to distill of IPA azeotrope, which will be recycled at reactor inlet.

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	Reactur Recyclet IPA area naterial balar	Reactor Separation Reactor Separation Recycle. IPA - Recycle. IPA - Recycle.

Now, we can very easily draw the recycle structure of this particular flow sheet, we have first the process or the reactor the feed to the reactor will be the fresh IPA azeotrope. Then the reactor effluent should enter a separation system product hydrogen can be taken out, because it is not a reversible byproduct. So, hydrogen can simply leave the separation system and can be used elsewhere the two products acetone and water, and leave the separation system.

There will be one recycle stream containing IPA azeotrope, which will be mixed with the fresh feed. So, this is a simple recycle structure of the flow sheet, we have determined it from theoretical considerations. We have to determine the recycle material balance the total IPA feed, which is at the reactor inlet which is the mixture of the fresh and recycle

feed. So, the total IPA feed we denote as FIPA. FIPA is equal to the fresh feed IPA that we denote as FFIPA divided by the conversion. Now, this is a relation that we have used earlier in case of HDA process as well. So, this directly applies in the present case, then we can easily if we substitute all the values that we have FIPA the total feed of IPA should be 100 divided by 0.8, which is a per pass conversion and that is 125 mole per hour.

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IPA in reycle stream: FIDA (1-2) = 125 (1-0.2) (Assumption: complete IPA necessary with no (0220) the in recycle stream : 0.3 x 25 = 10.7 mill (Assumption: The seems histillation column distills Mf 70% ItA azeotrye) Total veryde stream = 25+10.7 = 35.7 and

The IPA in recycle stream it will be obviously the unconverted IPA we have assumed complete recovery of IPA no losses. So, IPA FIPA into 1 minus x, so 125 into 1 minus 0.8 that turns out to be 25 mole per hour. I write here the assumption that we make complete IPA recovery with no losses. Now, this is the amount of isopropyl alcohol in the recycle stream, but the recycle stream is not pure isopropyl alcohol, but an azeotrope.

So, there will be definitely some water accompanying this particular IPA. Now, we assume that in the second distillation column. We can distill off IPA to the azeotrope level that is up to 70 percent of IPA. So, then H 2 O in recycle stream here, also we write the assumption that the second distillation column distills of 70 percent IPA azeotrope. With this assumption we can say that the amount of water in the recycle stream will be 0.3 by 0.7 that is 10.7 mole per hour. Now, we have determined the amount of sorry, the material balance of the recycle stream, so the total recycle stream will be 25 plus 10.7

that is 35.7 mole per hour. So, that point we note here 35.7 mole per hour of the recycle stream.

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· 7.2.9 Reactor Heat Ettect. reactor operates Assunino me ten and ettlue 25800 × 100 ad -2580000 Bh conde OT = 600 - 5R = 25" erce_ 8h 10 9 ...

Now, the third question was about the reactor heat effect the reaction is endothermic reaction. Then we have to supply the heat of reaction assuming that the reactor operates isothermally, which means that the temperature of feed and effluent form. The reactor is same, we can easily calculate the amount of heat that is required are given the tem temperature of feed as 572 degrees Fahrenheit. Therefore, the net heat load will be 25,800 into 100.

This is BTU per mole and 100 mole per hour of reaction. So, this is 25,000 8 0 0 0 0 BTU per hour. So, this is a reactor heat load, we are given the temperature of feed as 572. We assume isothermal operation that means the temperature is same the rector inlet and outlet and the dowtherm vapor condenses at 600 degrees Fahrenheit .This was also given to us if we assume no sub quilling of the condensate, the driving force or delta T will be 600 minus 572; that is 28 degrees Fahrenheit.

Now, we have not been given the overall heat transfer coefficient. If we have to use the relation q is equal to U A delta T, we do not know right now the U. However, if we have a vapor system; that means in the in a shell and tube heat exchanger, let us say one pass each one shall pass in one tube pass and vapor is reacting reaction in vapor phase is occurring in the tubes.

There is heat, a vapor condensing in the shell, the typical heat transfer coefficient that you are likely to have is something like 10 BTU per feet square per hour per degrees Fahrenheit. Now, this value I have obtained from the order of magnitude heat transfer coefficients given in standard text like, for example, Perry's a hand book or the book of Holman heat transfer or the book of D Q Kern process heat transform. So, for these kind of systems a typical heat transfer coefficient is given and I have taken the value of U from this text, okay?

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Dide Port O D Strame . Z. 1. J. J. S. P. - 2580000 -9214 84 Annual Full Lost ulnace efficiency , 60 %. at losses = 20% -\$ 5000 Fuel Cost = MMETU timal hours a 2580000 5,315,000 × 8000 -8000 ninace MMBTU 000

Substituting now all the values that we have are A is equal to q divided by U delta T q, we have just determined as 2.558 million BTU per hour, U is 10 and delta T is 28. We get the total heat transfer surface as 3214 feet square. So, that answers our fourth question. Then the last question the annual fuel cost from this area, you can also get the cost of the heat exchanger reactor, but that point we are going to deal in the other module of process economics in which we shall see the cost correlations.

So, that point we, I differ for the next module annual fuel cost, we have to determine. Now, the dowtherm liquid is evaporated in a furnace. Those vapors are transported to the reactor and then the vapors condense in the shell. So, there is in the first place the furnace efficiency comes into picture. Then the heat losses we have been given furnace efficiency as 60 percent heat losses as 20 percent. So, and the fuel cost is rupees 5000 per mm BTU metric million metric BTU and total operational hours as 8000. The reactor heat load is 2.58 million BTU that we just determined. However, the heat that needs to be generated at the furnace will be this divided by 0.6 into 0.8 because 20 percent will be lost. So, this divided by 0.8 into 8000. So, the total heat that needs to be generated or this I will heat generated in the furnace will be 53755.375 million BTU into 8000. This million BTU per hour into 8000 hour per year, so the annual heat will be 43,000 mm BTU and then the fuel cost will be.

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Fiel	Lost :	₹ [43,000 MMETU × SPITO] = 25,000,000 ₹ 21.5 (rove.

43,000 mm BTU into 5000 that will be 215million or Rupees 21.5 crore. So, this is how we have solved the problem of flow sheet synthesis for the IPA process. These are obviously very preliminary calculations in the subsequent lecture. We shall see more detailed calculations, especially the calculations of distillation column and the feed to effluent heat exchanger, all those thing.