Plant wide Control of Chemical Processes
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Lecture - 34
C4 Isomerization Process Case Study

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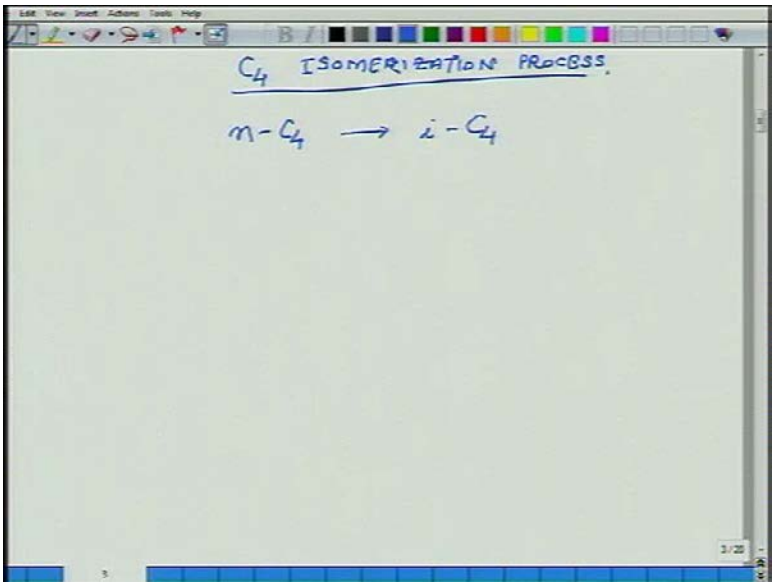

This is the isomerization process. In the refining industry, isomerization process, c 4 isomerization process, in the refining industry normal butane versus isobutane which one do you think is a more valuable feedstock.

(( ))

Why? Why isobutane is a more valuable feedstock? Branch chains are preferred, because branch chains can be used they do they can do a lot of chemistry. And branch chains when you add to petrol, octane number goes up right. So, between n c 4 and i c 4, i c 4 is preferred; i c 4 is more valuable. i c 4 meaning isobutane normal butane isobutane. So, you have a process which is basically isomerizing a to b, n c 4 to i c 4. And now what we have is the process looks something like this. You got a very tall tower we will make it and then may be if we have to redraw, we will redraw it.

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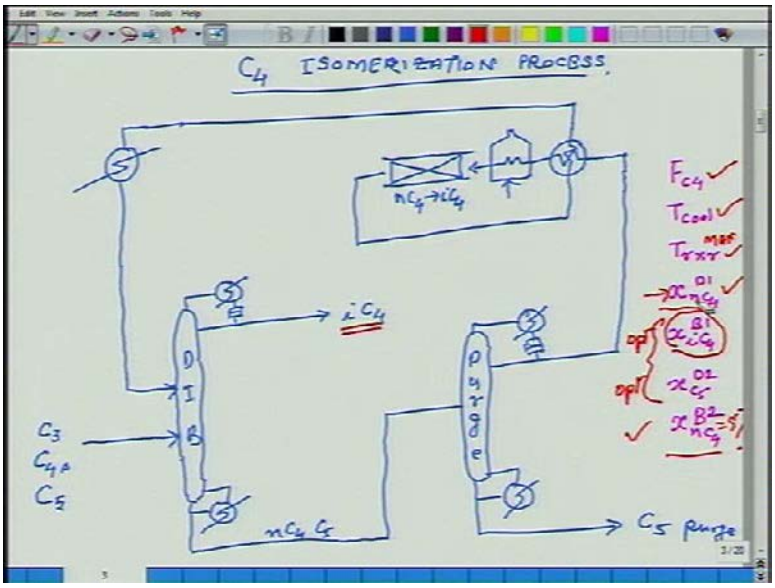

So, there is a de isobutanizer; it is a tall tower. You see i c 4 and n c 4 will be close boiling, because they are isomers; the boiling points will be very close. So, if you separate it using distillation, since the boiling points are not very different. You will get a very tall tower relative volatility is close to 1, may be 1.05, may be 1.1. So, you will get a very tall tower to separate n c 4 from i c 4. So, you take a stream which is the feed stream and the feed stream has got what? It has got some amount of propane, small amount of propane it has got the c 4, it has also got some amount of c 5.

This is a feed stream coming from up upstream. Isopropane is lighter than n propane, isobutane is lighter than n butane. So, you take out this is i c 4 comes out the top this is your product any c 3 that is coming in the feed is bound to end up at the top because c 3 is lighter than c 4. n c 4 and c 5 with small amount of iso i c 4 leaking down the bottoms, and that small amount you see if the separation is easy the small amount may be 0.1, percent since here the separation is difficult this small amount could be 5 percent even 10 percent. So, whatever c 4 is coming in whatever i c 4 is coming in ninety percent of it goes up ten percent of it leaks down. So, the recovery in the bottoms or loss in the bottoms is ten percent. If the separation was easier this number this recovery could have been less than one percent, but here the separation is difficult. So, you will not have very impressive small numbers for leakage down the bottom.

Now, this n c 4 rich stream is taken to what? A purge column. What does the purge column do, the purge column is a small tower. What it does is takes out the c 4 up the top, c 4 go up the top, the c 5 go down the bottoms; c 5 purge. The c 4 are now sent to a reactor after pre heating. Pre heating in a heater or a furnace I do not know. So, what you do is, you take this c 4 stream, you take this c 4 stream send it through a feed affluent heat exchanger, then send it through may be a furnace or may be a heater that depends on what the reaction temperature is. If the reaction temperature is above say 250 degree Celsius, you will have to have a either dove thermal based heater; if it is less than 250 degree Celsius you can use high pressure steam. If it is above 350 degree Celsius you will probably be using a furnace.

So, I am just may be making a furnace. The furnace is doing what, is heating the reactor to a heating. The reactor feed stream to its inlet temperature the reactor feed stream is then sent to what, a packed bed reactor which is adiabatic. What do you mean by adiabatic? Neither heated nor cooled. No heating, no cooling, it goes to this reactor in the reactor n c 4 reacts to give i c 4. So, this is the heating stream. So, I take this take it down. So, the cooled reactor effluent is further cooled and condensed in a condenser.

This stream, the outlet from the condenser is liquid. What you think would the composition of this stream be compared to the feed, in terms of n c 4 and i c 4. Let us say the fresh feed which is this guy, let us say it is 70 percent n c 4, 25 percent i c 4 and the rest is c 3 and c 5, 5 percent is c 3 and c 5. What you think the composition of this stream would be, what is coming out the condenser. So, the feed stream is rich in n c 4. What would the composition of the stream coming out of the reactor be, it would be rich in what n c 4 or i c 4.

Given that it is richer in i c 4 given that i c 4 is what is being recovered in the deisobuatnizer as the distillate, where should I be feeding it? Should I mix it with the feed stream you see, I could do this I am just you know talking for the heck of it. I could do this just mix it and send it to the deisobutanizer is that a good idea or is that not a good idea. Why is it not a good idea? (( )) the pation is not easy. So, we would not be able to recover back I mean.

But I, need to recover it. I have converted n c 4 to i c 4; some n c 4 is still remaining, I want to recover i c 4. And now my question is what is the best place to feed it in the

deisobutanizer. This is the deisobutanizer, and this is the purge column purge. So, where should I be feeding it, is this ok.

Student: Above

Why above?

Student: (( ))

Exactly, exactly that is all, that is all that I was asking. Where above sure you need to do an analysis, what is the best location, but at least this much should be clear that if I am mixing it with the fresh feed, I am something dead wrong. So, this is probably fed some place here may be. Does the process look ok? What is the steady state operating degrees of freedom?

Student: Seven.

Seven? How is it seven?

Student: Two plus two plus three.

Well of course, 1 plus 1 plus 1 plus done 7 times is also 7. Please give me an explanation.

Student: Two for the first column.

Two for the first column.

Student: Two for the second

Two for the second column,

Student: One for the furnace

One for the furnace

Student: One for the condenser

One for the condenser - the cooler you know, the this chap and one for the fresh feed.

(( ))

Well, furnace is reactor is adiabatic.

(( ))

See, that is why I asked the question. Reactor is adiabatic. There is no cooling. So, the only thing you can set is how much heat you are putting in the furnace, so that what is the temperature of whatever is going into the reactor. So, you does that make sense or no? So, that is that one degree of freedom that you have what is the temperature of the feed going into the reactor. Once it goes into the reactor, as much the reaction as has to happen happens, and then the temperature rises a little bit, and then the exit temperature is whatever it is. It is not a degree of freedom, because that is not in your hands.

Once you have set the reactor feed temperature, basically the outlet is fixed, well I need to qualify that. Once you have set what is going into the reactor that; that means, what is the composition, what is the temperature, what is the flow rate, what comes out gets set, yes or no? Temperature is getting set by the furnace, flow rate and composition are getting set by what you are feeding, how you are separating etcetera. So, what is flowing into the reactor is set by, whatever is the fresh feed its composition that is given. Then how much of whatever you are feeding goes up the top, how much of it goes down the bottom; then in the second column how much take down the bottom and therefore, what goes up the top that sets the flow rate.

What sets the temperature of this (( )), what sets the temperature of this chap - the cold feed to the reactor to the reaction section. What sets the temperature? Due point of the vapor at the column pressure, at the purge column pressure what is the due point of the vapor that is coming in the purge column. What sets the composition is basically how much you are removing that sets the composition in the flow. Furnace has been installed, so that you can have what is going into the reactor at whatever temperature you desire - that is the degree of freedom for the furnace. So, two degrees of freedom for the column de isobutanizer, two degrees of freedom for the purge column, one for the furnace, one for the cooler, and one for the fresh feed, so 2 plus 2 plus 2 plus 1 that is 7.

Now I ask start asking you questions.

Student: Sir, why I am taking for cooler? (( ))

What does the cooler do?

Student: Sir, vapor cool down.

And then it should do what?

Student: (( )) liquid

Exactly, and that liquid get set by what? Whether it will liquefy or not? You have to be in the two-phase region or in the sub-cooled region. And then you have to remove as much heat as is necessary to condense it out if you are removing less than that it will not condense. So, the need for condensation sets how much heat you need to remove yes or no therefore, you may decide not to count, it by saying that look the temperature is reasonable and it is dictated by the vapor liquid equilibrium just like you. Ignore the pressure inside a distillation column, you could ignore this too by saying that this temperature is something reasonable that will ensure that whatever is coming out the reactor condenses and liquefies, then you can discount it agreed. So, if I am counting it then my specification will be what the cooling duty should be. So, that my temperature is I do not know what may be 90 degree Fahrenheit 40, 50 degree Celsius fair enough.

So, I have counted it and then I have accounted it as a set point or temperature of the condenser outlet. So, the condenser duty is being set by the requirement of having the condenser outlet at I do not know 40 degrees 50 degrees. So, I have counted it, and I will account for it this way before I start drawing control system around it let us say I have designed this process to process some fresh feed rate let us say 100 kilomoles per hour of fresh feed. I have designed this process for that, and now I want to run it in the most efficient possible way.

So, my fresh feed rate is given that takes care of one degree of freedom, I count it seven one degree of freedom gets taken care of my fresh feed rate is given. We just argued that the temperature at the outlet of the cooler should be reasonable. So that everything condenses right as long as it is reasonable, it will not have much of a role to play in terms of optimal operation, so that takes care of two. So, what I am saying is let me just write it here. What is given and what is accounted for and what needs to be. So, f c 4 is given fresh c 4 that is coming is given temperature of the cooler is set at a reasonable value. So, out of the 72 are taken care of. Now I am left with 5 degrees of freedom, what are they

two separations in the column, 2 plus 2, 4 and inlet temperature of the reactor, reactor inlet temperature these are the 5 degrees of freedom that are left. Steady state control system will come to later first let us just understand how do I adjust these 5 degrees of freedom. So, that my operation is optimal that is the question now think about it and tell me. So, what I am saying is temperature of the reactor what should i do with that what would be reasonable de is you know specs on d i b and purge columns there are two specs on the d i d isobutanizer.

There are two specs on the purge column, what would be reasonable values for them, what would be reasonable specification variables for them, what the hell is the rectifying section doing in the deisobutanizer said is butane. We have done and I want the specific answer, it is separating and understood. What is the light key and what is the heavy key in the deisobutanizer, what is the definition of a light key and height and a heavy key? What does the rectifier do a rectifier prevents the heavy key from leaking up the top anything lighter than the heavy key. Essentially goes up the top yeah what does the heavy key do what does the stripping section, do it prevents the light key component from leaking down the bottoms anything that is heavier than the light key essentially goes down the bottom.

So, the split is a light key heavy key split yeah. So, what is the split in the d is botanizer I c 4 n c 4 it is got nothing to do with c 3 c three any c 3 is there is bound to go up the top because its lighter than the light key. So, now, I rephrase again the same question what is the rectifying section in the deisobutanizer doing? It is preventing n c 4 from leaking up the top. So, reasonable specification variable would be what the mole fraction of n c 4 in the distillate is of what, deisobutanizer that is one. What is the next specification? There are two specifications for the column. For the deisobutanizer column, we have specified what the rectification section of the d i b must do. What is the stripping section doing? preventing i c 4 from leaking down the bottoms. So, I say x i c 4 down the bottoms, so 1, 2, 3, 4, 5.

Similarly, two specs for the purge column, what are the rectifying and stripping sections in the purge column doing? The function that they are accomplishing.

Student: Sir, in purge column rectifying section preventing the n c 4 and c 5.

No, no

Student: n c 4 only

no

Student: (( ))

Preventing the c 5 from going up the top. If there is any n c 4, the whole idea of the process is all the n c 4 convert must be converted. If I take if I do not allow the n c 4 to go up the top nothing goes to the reactor. Only if it goes to the reactor, if in the purge column I make sure that the n c 4 does not go up the top, then what have I done? I have taken it all out down the bottoms right. So, what is the rectifying section of the purge column doing, it is preventing c 5 from leaking up the top. So, I would say x c 5 may be we will call this d 1 b 1 first column and will call this d 2 second column distillate

And what is the stripping section doing, preventing what? i c 4 or n c 4 or both. Key component will only be one either this or that.

Student: n c 4

n c 4, why?

Because, n c 4 is the heavier one and that is what I am preventing from going down the bottom anything lighter than n c 4 is guaranteed to go up. So, x n c 4 d 2 sorry b 2. These are my seven specs, I just argued this is given this is what, basically it should be reasonable, so that everything condenses I am not going to fuss about it. What about i c 4 there must be some purity constraint on the i c 4. Basically I am saying this is a product purity spec. The amount of n c 4 impurity in the i c 4 must be below, let us say I do not know 2 percent may be 5 percent.

So, this is a product purity spec, I would not like to over purify. Yes or no, why is that? Let us say, I want only two percent; let us say my spec is that n c 4 in the distillate should not be should be less than 5 percent. Let us just say it is this. I can operate at exactly 5 percent or I can also operate at 4 percent or may be three percent, less than constraint is satisfied. Where would I operate? obviously, you will say, I will operate at 5 percent. Why? Extra purification is going to cost money.

Student: (( ))

Well, something more than that more important than that. Let us say you are allowing more n c 4 to go up the top. The reason is this is called the avoid product give away rule. If I am allowing my product to be over pure; that means, impurity is less; if impurity was supposed to be 5 percent, let us say I am having only one percent impurity. What is that means, is the impurity does not fetch me anything – price. If I send maximum impurity, maximum impurity that is allowed in the product, I am getting paid for the impurity. What am I getting paid for paid for the impurity, I am getting paid the price of the product yes or no? Therefore, it is always economically optimal 99 percent of the time to basically have your product purity at the constraint, and not over purify because that allows you to sell something that is cheap for the price of something that is expensive yes or no? Basically, in not so simple terms is cheating - legal cheating.

When we came at the purity of the product is 95 percent the that is suppose that for that only we are getting paid

But, when I am saying I guarantee you that it is octane number is 87 and let us say I am actually selling petrol that is 91 or 95 octane number; that means, that means I am adding extra branched yeah right, but I am getting paid only for 87, what I am selling is 95 octane. I am acting adding extra additives; am I fool yes or no? Every businessman knows this, adulterate to the extent allowed yes or no? That is what it is. So, therefore, this which is the quality spec on the product must be at its constraint. You must allow maximum amount of n c 4 to leak out as much as is allowed. If it is 5 percent, 5 percent; if it is 2 percent, 2 percent whatever. So, we cannot argue about this. So, this is also set, now we are left with what 4 things. I can clearly see that if I allow n c 4 to leak down the bottoms in the purge stream n c 4 i was wanting to convert to i c 4, n c 4 has leaked out that much less i c 4 i generate that is that will represent loss in revenue.

So, most certainly this (( )), this chap here the mole fraction or the amount of n c 4 leaking in the purge stream, in the c 5 purge stream must be kept small. We can argue how small, but nevertheless it must be kept small. So, let us say I keep it at I do not know may be 5 percent. Why 5 percent, because you may say 5 percent is large I am saying well c 5 is anyway in small amounts in the feed stream. So, let us say if you are putting in hundred kilo moles of the fresh feed in that c 5 will be two or three kilo moles. In two or three kilo moles of c 5 if you allow 5 percent n c 4 to go out how much would that be?

Student: (( ))

Something like that right, very small pretty small. The point is this purge stream flow rate is small, and so you can allow I am not going to fuss about is it with the 5 percent or ten percent, basically, you have the awareness that you cannot allow too much n c 4 to leak down. And let us just say I am saying 5 percent is what I call too much, so that takes care of this. Now I am left with what, what should I do to the reactor temperature.

Student: It should be some optimal values.

Should be some optimal values, of course.

More temperature will lead to cracking of n c 4.Cracking. So, as high a temperature as possible. Whatever that as high may be, why as high?

Student: (( ))

Exactly, if the temperature is as high as possible, basically the recycle stream goes down. If conversion is as high as possible, un-reacted n c 4 is small; un-reacted n c 4 is small means the n c 4 recirculation in the recycle loop is small. If n c 4 circulation in the recycle loop is small, essentially both the boil ups actually go down. The boil up in the deisobutanizer goes down, the boil up in the purged column also goes down. So t reactor should be max.

Now I am left with what, and this max could be you know pros people say that look if you if you go beyond this temperature like this fellow says c 4 starts to crack. Or you know the maximum temperature allowed for this catalyst is this beyond this temperature, the catalyst starts to centre, coke starts to deposit, it starts to lose activity, we have to shut down earlier and replace the catalyst blah blah blah. There might be you know from processing constraints, you will have do not operate the reactor beyond this temperature. Well that temperature is what I operate at. So, that is t reactor max.

Now I am left with two thing, what are those two things? Those two things are these, these two chaps. And what do they represent, x i c 4 in b 1 in the bottoms.Whatever is the i c 4 that is leaking down the bottoms, and x c 5 in that distillate from the purge column whatever is the c 5 that is leaking out the top. What does this represent, what do

these things represent? These things represent the i c 4 circulating around inventory of i c 4 circulating around, and inventory of c 5 circulating around, yes or no?

Now that I have said this what do you think should be done with these two things. Can I say that this should max, min this that etcetera.

Student: Because, they are wasting energy in circulating.

No, it is the other way round actually if I have see, separation in the deisobutanizer is hard, so if I allow more i c 5 to leak out, what happens? Boil up will go down, my steam consumption will go down. What is the problem with this, the problem with allowing more to leak out is whatever is leaking out, whatever i c 4, i c 4 is leaking out in the purge column it has to be sent up; you to boil it and send it up.

So, the boil up in the d i b goes down, boil up in the purge column goes up. You can clearly see there is some optimum you cannot really clearly tell which way, but I can most definitely tell, because the boil up in the d i b is going to be large, because it is a tall tower separation is harder. Most certainly I must ease out on this, this must be relaxed not be too tight, because the moment I start making it too tight, what will happen is the boil up in the deisobutanizer will shoot up exponentially. What is that number 5 percent, 10 percent I do not know, but at least I know it cannot be too tight it has to be on that side.

Student: Sir, on the second column, the first column why would increase i c 4 increase the boil up I mean they are…

What is the state of the i c 4 that is coming out here? It is liquid

Student: Yeah.

Ok.

Student: But, sir when we are ensuring that the n c 4 goes up the bottom i c 4 will automatically…

Yeah, but how does it go, it does not go automatically.

No, if we are boiling I mean the energy required to boil that much amount of n c 4.

Forget that, let us say I have got n c 4 and i c 4; n c 4 is being boiled up, i c 4 is lighter i c 4 is lighter than n c 4. Now, let us say the for the same flow rate, well not for the same flow rate. Let us say component flow rate of n c 4 is fixed - component flow rate, i c 4 component flow rate goes up. What will happen to the boil up? It will go up right? You have to boil up any way you have to boil it some energy will get taken for that; however, because that separation is easier on the purge column.

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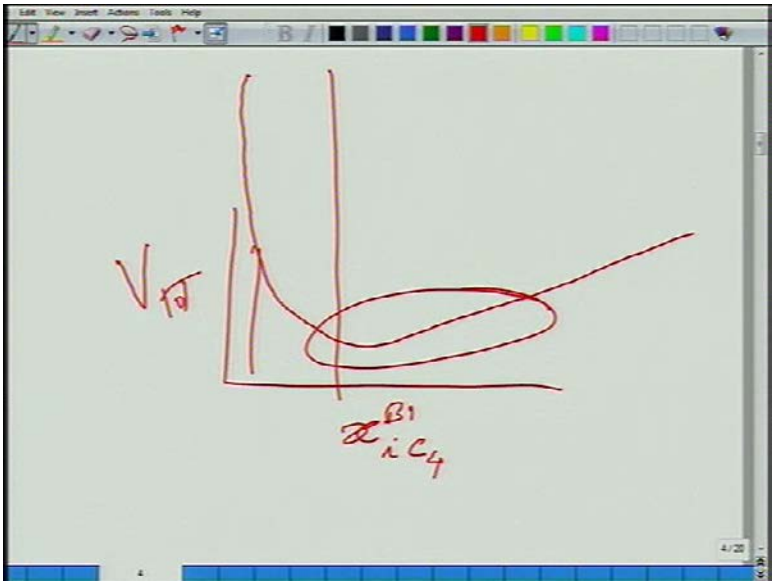

What do, what I expect is if I look at, for example, the boil up curve, if I look at the boil up curve and I am plotting x bottom in bottom 1 of i c 4 right, i c 4 was leaking down the bottom. I can clearly see that if I look at boil up total; that means, the boil up in the first column and the boil up in the second column. If I look at these two things total sum it up. What I would probably find is a curve that looks something like this. You see below this, there is a sharp rise in boil up, because beyond this the rise in boil up is there, but it is not a sharp because the second column separation is much easier I can you know this I can see qualitatively.

So, as long as I am somewhere here, I am ok, you see what I am saying. So, I may say I would say may be 5 or 10 percent of i c 4 leaking down the bottoms, one percent would be too tight I will be somewhere here. Does that makes sense or no? What exactly I do not know. Reasonable value I can guess, exact value I can get from an optimization like this. You know exact value will be this guy where you have minimum. So, I this will

have an optimum; this will also have an optimum, but the point is just looking at the process, I have been able to figure out what I need to do with degrees of freedom. What are the reasonable things to do with to manage my seven degrees of freedom, yes or no?

No mathematics, no nothing just common sense. Where do I need to apply some amount of analysis, probably to figure out what to do with these last two remaining degrees of freedom. Where I really do not know exactly what should be the set point. So, that my boil up is minimized total boil up is minimized total energy consumption for the same throughput is minimized. But I do know I can be near optimum by applying simple common sense, yes or no?

Now that I know this, next class we will worry about maximizing throughput. What do I do, so basically what I am saying is I have got two unconstraint degrees of freedom for a given throughput. If I am wanting to allow the throughput to be maximized; that means, throughput itself is a degree of freedom, then I have three unconstrained degrees of freedom. If three constraints become active, I would have lost all degrees of freedom and then my throughput is maximum, and once we have seen that we will implement a control system.