Aspen Plus Simulation Software – A Basic Course for Beginners Prof. Prabirkumar Saha Department of Chemical Engineering Indian Institute of Technology, Guwahati

Lecture - 32 Isobutene Production Plant

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Welcome to the massive open online course on aspen plus. In today's lecture we shall perform a case study on isobutene production plant. The problem statement is something like this, the isobutene will be produced from isobutene flowing at 125 mol/hr25 0 C and 5 bar pressure; this is a high-pressure operation. The stream is first preheated to 600 0 C.

So, from 25 0 C to 600 0 C and fed into a catalytic PFR plug flow reactor and that plug flow reactor operates at 600 0 C and 3 bar pressures. So, it is entirely vapour phase operation it follows the reversible reaction of class LHHW. LHHW means it is Langmuir Hinshelwood Hougen Watson. So, this is the model and the reaction rate of that class of model is given as follows.

Where this is the driving force option and the denominator is the adsorption option so basically it relates the adsorption with driving force in the reaction rate. So, this is the reaction this is isobutane this is isobutene and, in the process, it loses hydrogen. So, in the bargain we produce

hydrogen. Now in this reaction rate we have this data, the K is given by this K capital K, keh and ke all of them are given.

Now here the suffix a is given for isobutane and suffix e is given for isobutene and suffix h has been given for hydrogen and when both hydrogen and isobutene is there to denote that we write eh both the suffix together. And this reaction the basis is partial pressure sometimes we can choose basis as concentration but here we are choosing the basis as partial pressure. And here you will find the e term that is the activation energy the unit is kJ/mol.

And R value has been given generally R value we write in J/kmole k but here we are writing it in meter cube bar k mole and the value is this. So, we will use this value while doing the calculation. Now the PFR has 12 tubes and each one is 450-centimetre-long 10 centimetre in dia, and is a catalytic reaction. So, we have loading of catalyst 1.2 kg of catalyst with 60% bed voidage. So, we will have the pipelines which are loaded with catalyst and 60% of bed voidage.





So, basically, we have the feet this is preheated and this is sent to a PFR. So, feed is at 25 0 C and 5 bar pressure and here it is preheated to 600 0 C and 3 bar pressure and this is the reaction condition in PFR. The PFR configuration has been given so here up to this point. (Refer Slide Time: 05:39)



Now the outlet of the PFR is cooled to 85 ^oC before it is passed through a membrane separator where hydrogen is completely separated the remaining mixture of isobutene and unreacted isobutane is terms as REST. So, this is first cooled to 85 ^oC and then it is passed through a separator where pure hydrogen is separated from the REST and this REST contains unreacted isobutane plus the product that is isobutene

And 80% of the REST is recycled back to the PFR after necessary temperature and pressure correction. So, this one we will split and 80% of that will be recycled back to the PFR and obviously that will be done with some temperature and pressure correction. So, we know for pressure correction we have to use a compressor and for temperature correction we have to use a heater.

So, after doing that we can send to a mixer and that will mix it with the original feed. So, this is the complete picture till. Now then we have to replace the preheater with a shortcut exchanger and optimize the heat duty. What does it mean? Here we were using a simple heater we have to replace this one with the heat exchanger and we have to compare the heat duty. We need to calculate the heat duty in this configuration and then we have to replace this one with a heat exchanger. And we have to cut this line take this stream to preheat this stream and then outlet of this we will pass to the heater. So, this is what we will be doing and whatever the temperature correction that we will do through this particular heater before sending it to the PFR. So, this is the complete picture now this 20% remains. Now what we have to do? We have to add a purifier for this 20% of the REST.

So, first we have to try a flash separator and distillation column and then we have to perform sensitivity analysis with reflux rate distillate rate, number of stages, condenser pressure. If they are successful, we are happy if they are not successful, we have to explore a membrane separator. So, that is our complete task we shall do this thing later first we have to do the preliminary part.

And then do the recycling and comparison of heat duty and this will come at the last portion. So, let us go to the aspen plus simulation window.

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So, first we have to add the components, first we have Isobutane this one adds it and then we will have isobutene this one so adds this and finally we will have hydrogen. So, we will say H_2 and these two we can replace it with say C_4H_{10} and this one we can write as C_4H_8 . So, this is isobutane this is isobutene. And we shall use Peng Robinson method so done now let us go to the simulation window.

So, let us refer to our diagram. So, we need first we will use a heater then a PFR then a cooler and a separator. So, we will have a heater then another heater over here that we will use as a cooler and then we will have a PFR let us use this icon and we will have a separator. So, let us rename them first let us write as H1 this is PFR this is cooler 1 and this is separator 1 so, H1 PFR C1 and sep1. Now connect the material streams, now we have to rename them.

So, let us rename it as feed this is H1 out this is PFR out this is C1 out this. This will be pure hydrogen because we have to separate pure hydrogen from the product stream and this will be rest that has been named in the problem statement itself. So, what is the feed condition? Please

refer to feed condition. This is one 25 kmole of Isobutane 25 0 C 5 bar pressure. So, we will have the feed condition.

It is 125 kmol/hr 25 0 C and 5 bar pressures. Then we have to fix the heater will be 600 0 C and it will be 3 bar pressure, so this is 3 bar pressure outlet. And then we will fix the PFR later then C1 it will come out at 85 0 C and there is no pressure drop. You can refer it is said that the outlet of the PFR is cooled at 85 0 C, before it is passed through a membrane separator where H₂ is completely separated.

So, we shall have the separator, this outlet stream H_2 will have complete H_2 all others will be 0. So, that is the separator 1. Now we have to fix PFR. Now before fixing PFR let us go and set the reaction. Now always go and start with a general reaction and then go towards LHHW, that is Langmuir Hinshelwood Hougen Watson. So, we start with a general reaction type. So, press new. This will be a reversible reaction as it is mentioned.

And this is LHHW give a name to the reaction say RX. So, here the reaction is; let us refer it once again before we go forward. So, this is isobutene converts to isobutene and hydrogen. So, isobutane converts to isobutene and hydrogen. Now we have to take care of the kinetic information. So, reaction is reversible reacting phase it is vapour phase it is mentioned over here. This is an entirely vapour phase reactor and everywhere we have this pa, pe, ph.

So, our CI basis will be partial pressure and we will use it as bar. And here it is a catalytic reactor so we will give the weight of the catalyst and the rate will be calculated on the basis of at catalyst weight. Now we have to give this information. So, here t 0 is not specified so, k will be $8.9*10^5$. So, 8.9 E5 and E will be 112 kJ/mol. So, this is 112 kJ/mol. So, this is done.

Now first let us understand the adsorption part then we will do the driving force reaction rate unit we will use it as moles/gm*sec because everywhere we are using moles. Now absorption terms we have to give as term 1 term 2 term 3 etcetera where term i, i means 1 2 3 etcetera. That will be ki $*c^1$ to the power n1* c2 to the power n 2 and so on. But in our case, we have got this is our term 1 this is term 2 and this is term 3.

And in our case, we do not have the basis C we have the basis of partial pressure. So, kh will be in our case term 2 it will be ki, pi 1 to the power n 1 i to the power n 2 etcetera. So, we have to write it in that form this c1, c2 etcetera. So, we have three terms so, this is for component butane and this is for hydrogen. Term one we have 0 because we do not have any concentration exponents term 1 is 1 only there is no concentration exponent over there so we write 0 term 2.

We have concentration or pressure exponent one for both pe to the power 1 and ph to the power 1. So, we have both 1 and 1 and term 3. We have concentration exponent of only isobutene not hydrogen. So, we shall give only for butene this is one for hydrogen there is nothing 0 and adsorption expression exponent this is also 1, because at the denominator the whole term is 1. Now term one, what is term one?

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We have to give this information to aspen plus in the form of $\ln k I$ mean whether it is, ka, ke, kh anything $\ln k$ will be A + B by T + C $\ln T$ + D into T.

$$\ln(k) = A + \frac{B}{T} + C\ln T + DT$$

So, it will be in this form so all of them we have to convert it in this form. So, in the first case for keh it will be ln k eh will be ln of 1.2 into 10 to the power 6 + -79 by r. So, it will be -79 by 8.314 into 10 to the power -5 by T + 0 + 0. So, C and D will be 0 for this particular expression.

$$\ln(k) = \ln(1.2*10^6) + \frac{-79}{8.314*10^{-5}}$$

And this one will be A this one will be B and if you calculate your A will be 13.9978 your B will be -950204. So, we have to enter these two terms in aspen plus so just go to aspen plus window.

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So, for term one when it is equal to 1 then A = 0 B = 0 C = 0 and D = 0. So, for all of them we will have 0 only. So, k1 so term 1 = 1 and term 2 as we have calculated just now it will be 13.9978 and B will be -950204. So, just see it has come in this fashion so k2 = 1.2 into 10 to the power 6 then e to the power - 79 by r, so 79 by r is this one only. So, similarly the third term it will have this one.

So, it will be A will be ln of $2.5*10^5$ and B will be $-87 / 8.314*10^{-5}$. So, if you calculate that your A will be 12.429 and this will be -1046428 so insert these two figures into aspen plus simulation window. So, your A = 12.4292 and this one is - 1046428. So, this is done. So, all the three terms have been given so you compare your rate expression this kinetic factor driving force and adsorption.

So, we have already fixed up the adsorption and kinetic factor k and we have to give the driving force now. So, for driving force we already have the data with us. Here it is simply one will directly give these values specify rate constant and concentration exponents for forward and reverse reaction. So, for forward reaction exponent is 1 because it is only p a and for this is 0 and this is 0 and all the coefficients are 0 as well.

And for reverse reaction it is pe, ph by k so, there will be no reactant over there for products there are two exponents and here also the coefficients of the driving force are like this. So, we

have set the reaction done. So, r1 we have fixed now go back to PFR. So, setup PFR the reactor operates at constant temperature of 600 0 C. So, reactor with specified temperature of 600 0 C.

The configuration it is a multi-tube reactor it has 12 tubes each one is 450-centimetre-long and 10 centimetre in dia loaded with 1.2 kg of catalyst with 60% bed voidage. So, we have to insert this information. So, this is multi-tube reactor with 12 tubes the length is 450 centimetre and dia is 10 centimetre and the reactions already we have defined just press it over here pressure it operates at 3 bar pressures, PFR operates at 3 bar pressure entirely vapour phase.

And then catalyst. Catalyst is 1.2 kg of catalyst loading is there with bed void at 60%. That is how we specify the PFR, now everything is set. Let us run. So, the run is complete just click the temperature, pressure and molar flow rate. So, 125 was the molar flow rate at the inlet and we have got 188 of molar flow rate in the PFR out. And we have got 62 kmol/hr of hydrogen this line will be full of hydrogen.

And that is how the separation unit has been designed. So, here we have only hydrogen 62.5 kmol/hr and the rest it will be only isobutene and isobutane unreacted and thereof equal proportion. Now we have to take out 80% of this and recycle it back. So, what we need to do? We need to use a splitter over here and we need to use a mixer over here. So, first we make some room for this one.

So, we reconnect destination to mixer and we connect this with this then we connect this with this and this is the 20% of REST. And we have to recycle it to the PFR after temperature and pressure correction. Now let us see what is the pressure over here pressure is 3 bar and here also pressure is 3 bar. So, there will be no necessity of any compressor over here. Now we shall change the simulation a bit because later we are going to replace this heater with a heat exchanger and calculate the change of heat duty.

Now this heater not only heats but it changes the pressure also. So, the total duty will be more than just heat transfer duty. So, what we will do? We will keep here as 5 atmospheres only and let the PFR do the job of changing the pressure. So, we shall make it 0 pressure drop split block

needs extra outlet. So, we will name them later and we have to set split fraction of 0.2 that means 20% to this side. Now it will run, now we have to do certain temperature and pressure correction.

So, for that we shall need one pressure changer over here and one exchanger not exchanger one heater over here and first we shall rotate the icon flip horizontally and this one also flips horizontal. Now connect this one at this end then connect this one to this end this, now let us change the name. So, this is our product this is recycle reconnect source at this point. So, this is compressor, this is heater 2, heater 2 already exists fine.

So, we are using H_2 for hydrogen so we have to write heat 2 this one is come out and this is to H is 2 out. Renaming is complete we have to assign the values in compressor. So, this is a compressor of type isentropic and the discharge pressure should be 5 bar. So, that it mixes with the line and this heater output we do not know what should be the temperature of the heater output.

So, let us say that our heater temperature is say $600 \, {}^{0}$ C and no pressure drop. So, if we run it now so the simulation is complete. Now we have to check the heat duty. So, we find the heat duty of H1 is this, PFR this, c1 this and He2 heat duty is this. So, this plus this plus this plus this so total heat duty this will be 7616285 so much of cal/sec. So, this much of heat duty will be required for running this process.

Now we have to replace this heater with a heat exchanger. So, the idea is that we are using one heater to increase the temperature from 25 0 C to 600 0 C, a cooler to cool down from 600 0 C to 85 0 C and another heater to increase the heat from 106 0 C to 600 0 C. So, why to use three heaters like this rather we can use some heat exchanger which can exchange the heat between two process streams.

And minimize the heat loss and save some money for heating. So, for that we have decided to replace this particular heater with a shortcut exchanger. So, this will be regarded as a preheater and later we have to optimize its heat duty. So, we replace this. First, let us cut this heater and

then insert a heat x. So, let us connect this cold stream this is called out and then we reconnect this stream to this destination and we connect these two ends. So, this is what we have.

So, we are using the heat of the process stream that is coming out from the reactor to pre-heat the feed. And whatever the temperature this stream will come out that will be corrected with this heater. Now obviously if our hot stream inlet is $600 \ ^{0}$ C then cold stream outlet cannot be equal to $600 \ ^{0}$ C it should be less than that. So, we will specify the cold stream outlet to be say $500 \ ^{0}$ C or $550 \ ^{0}$ C, run this.

So, it has converged, but there is one problem over here. It has decreased the inlet temperature of the reactor to 589. Although the reactor is operating at 600 0 C and that is the reason why this stream is coming out at 600 0 C. But the PFR is using its own heating mechanism in order to increase this temperature from 589 to 600 0 C. But we do not want that. We want the stream to carry material at 600 0 C itself.

Now this is with a temperature of 550 0 C and this heater is sending the stream at 600 0 C. So, this particular mixer will have a combined fluid which will have 589 0 C. Now what we need to do? We need to fix this temperature at 600 0 C by manipulating this temperature to whatever. So, we will use a design spec for that which will fix this particular heat temperature by manipulating this one.

So, for that let us rename it first let us rename it as heat x, let us rename it as mixer out. So, we want to fix the temperature of m out by manipulating temperature of h to out. So, for that let us use a design specification, press new. So, define amount temp which is a stream variable of stream m out the temperature is the variable. So, amount temp its target should be $600 \, {}^{0}$ C with a tolerance say 0 0 1.

And we will vary the block variable which block it should be He2 and the variable again it will be that temperature and obviously it will not be less than 600. So, let us start with 600 and end with say 700. So, we expect that the desired temperature will lie between 600 and 700 so this is

our DS1 fixed. So, run. Now it is done. So, just check the temperature becomes 614 $^{\circ}C$ that means if the temperature of He2 out is 614 $^{\circ}C$.

And H1 out is 550 °C then this mixer will send out a combined flow which will be of 600 °C temperature and this is the ideal temperature for the PFR to work. So, we have fixed our He2 out at temperature 614 °C and there is no need of design spec so we shall just deactivate this. So, run it once again done. So, we shall calculate this heat duty once again.

So, this is this much this one, this one and this one, so this plus this plus this plus this and the total will be 6761623 cal/sec. So, this will be the total heat duty by using the heat exchanger. Now compare this with this obviously there will be a reduction. How much? The reduction will be 6762623 by 7616285 into 100%. So, it will be 88.77% that means instead of using heater if you use a heat exchanger then you can save around 11.23%.

So, by using a heat exchanger in place of a heater we can save 11.23% of heat duty. Now our job is not over we have to optimize this heat. Now for optimization you can add up this particular stream plus this particular stream plus this particular stream plus this particular stream and join them all as the objective function. So, you can open a model analysis tool optimization O 1Q heat x it is a block variable.

Which block? It is the heat x block the variable will be the calculated exchanger heat duty. So, similarly so first let us copy and then paste, paste, paste. So, let us change it to PFR and all of them will remain same except in place of heat x you put PFR. This one renames it as c1 and in place of heat x you will have c1. And this one He2 in place of heat x it will be He2. So, we have defined the calculated heat of heat x PFR c1 and He2.

And remember this one is positive, this one is positive while this one is negative, this one is also positive. So, c1 is a cooler. So, we will use Q heat x + Q PFR – QC1 because is a cooler and + Q He2 so this one we have to minimize. And what we need to vary? We need to vary the cold stream outlet flow rate of heat exchanger. So, this will be block variable. Which block? The heat x which variable the cold stream specified outlet temperature of cold stream.

So, the lower limit we give 500 and upper limit we give 580. And as we will do the optimization, we still need the design specification. So, we will activate the design specification. We can fix this little bit higher and this is a little bit lower. Now let us run the optimization. So, it has rather converge very fast go to the result. So, it has reached 580. So, it has reached the upper bound. That means as you go closer and closer to $600 \, {}^{0}C$.

The total heat duty will be better and what is the objective function? The total is 6709519. So, it is even less than the figure that we had obtained before. Obviously, if the cold stream outlet temperature is higher that means the feed stream is preheated more. So, the load on He2 to correct the temperature of the combined fit will be less. So, the total heat duty will be less. So, this is quite expected and we are happy with the result.

Now we shall again deactivate design, spec will deactivate optimization. So, we have already done this one. So, now we have to add a purifier for the 20% of the REST. So, for that let us see what is there in 20% REST. So, just go and check this stream product and here we will find total 125 moles out of which 34.4 kmole is unreacted butane and 90.59 kmole is the isobutane the product. Now suppose we place a flash tank.

So, write flash here, it is FVAP this is third leak and the flash tank let us say its heat duty is 0 and pressure drop is also 0. So, if we run it. So, you can see the temperature is 85 $^{\circ}$ C and the entire material has gone up 125 kmole/hr. Whereas the bottom there is 0 nothing is there. So, let us change the temperature. So, with 0 heat duty do not work. Let us decrease the temperature to 50 $^{\circ}$ C.

And run it still everything is going at the top, nothing in the bottom. And check the temperature, let us cool down some more say 10 $^{\circ}$ C. Now everything has come down to the bottom nothing is at the top. So, let us do a sensitivity analysis from 10 $^{\circ}$ C to 50 $^{\circ}$ C and check how the fluid moves in the flash tank. So, go to the model analysis tool, sensitivity analysis, create a new.

And then we have to vary the temperature of block which block flash and what do we vary the temperature from 10 0 C to 50 0 C with an increment of 1degree, we will define the flow rate. So, vapour flow rate which is a molar flow rate of stream EVAP of component C₄H₈ and also, we will check another flow that is total flow. So, which will be a stream variable which stream it is FVAP, and what variable? The molar flow rates.

So, this will be a total flow this will be only the isobutene flow and we will tabulate both of them run, result is available check. So, from 10 $^{\circ}$ C to 23 $^{\circ}$ C there is no flow at the top. And at 24 $^{\circ}$ C everything comes to the top. So, let us fine tune say 23 to 24 so go to the sensitivity analysis. Once again check it from 23 to 24 run with 0.01 and run once again 100 points will be there.

Again, we see, so, from 23.27 to 23.4. So, within these 2 temperatures everything is going either top or at the bottom and really, we cannot control it because if the temperature is slightly here and there then either the entire thing will go down or it will go up. So, I do not think that using a distillation column or a separation column will help because the content is very, very sensitive to temperature.

So, I am sure that it will not work but still let us try once, let us cut this and replace it with a column say let us take a rad frag and let us connect this thing with this one this thing with partial distillate this thing with a flick. So, this is our column and we have to define various things at columns. So, let us use 25 stages condenser maybe partial vapour and distillate rate let us use 70 because we need 70 kmol/hr out of 125 kmol/hr.

Reflux ratio let us use three streams fix stream. Let us put at 12th stage and pressure let us operate at say three bar pressures let us not change it, because it is at 3 bar the reactor output and run. So, this is the result. If you want to run this column with the expected output you need to attain a temperature of 23.09 ^oC at the condenser and 23.7 ^oC the reboiler. Now you can very well understand that it is not possible for a 25 stages column.

To maintain in such a fine temperature difference that at the bottom it is 23.7 and at the top it is 23.09. So, the option of distillation column is at all not possible. So, in the problem statement it

is said that we can try out sensitivity analysis with reflux rate, distillate rate, number of stages, condenser pressure etcetera. We have tried flash separator it did not work. We tried distillation column and it seems it will not work.

But still, we can do some sensitivity analysis with these things. For that again we have to go to the sensitivity analysis tool. So, s1 so we will vary say reflux rate. So, it is a block variable which block it is column and which variable it should be reflux ratio. So, it is mole RR. So, molar reflux ratio and we have used reflux ratio 3. So, let us start from 1 and do it up to 5 with an increment of say 0.1 and check how the V flow and T flow work.

So, what is V flow? V flow is the molar flow rate of stream FVAP and component isobutene and T flow is this a stream variable of stream FVAP and the variable is molar flow and then we shall fill the variable tablet. Now run. So, it has run obviously this will come with lot of errors because it cannot work in that range, I believe actually errors are there at the first four cases so, from reflux ratio one to one point three does not work.

So, perhaps 1.4 is the minimum reflex ratio and that is the reason why the simulation is not possible for these for reflux ratios. Now never bother let us analyse. When it is 1.4 it is 48.7952 and when it is 5 it is 43. So, the kmol/hr does not change much. So, the purity of isobutene does not change much, it is 43 out of 125 so it is not much. So, we have tried with reflux ratio that did not work.

So, you can try with reflux rate, distillate rate, number of stages and condenser pressure because by now you have learned sensitivity analysis quite well. So, I will not do over here you can do it yourself as a practice. And I am sure that even by doing the sensitivity analysis you will not get any better result than whatever we have got just now through reflux ratio. So, in short neither flash separator nor a distillation column will be an ideal candidate for the purification of C_4H_8 from the mixture of C_4H_8 and C_4H_{10} .

So, only instrument that you can use is a membrane separate. Now by saying membrane separator obviously we do not have a proper model of a membrane separator. So, you can just

use a simple separator to separate them. So, basically you have to remove this one and place one membrane separator. And through that membrane separator you can separate C_4H_8 and unreacted C_4H_{10} .

And that unreacted C_4H_{10} you can recycle and check what is the increase in percentage of production of isobutane. So, that portion I keep it as a practice task for you. Because by now you might have learned many things about aspen plus. So, this portion it will be very easy for you to do.

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So, with that we come to an end of this case study and we will come back with another interesting case study in the next lecture. Thank you.