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

Lecture - 33
Nitric Oxide Production Plant

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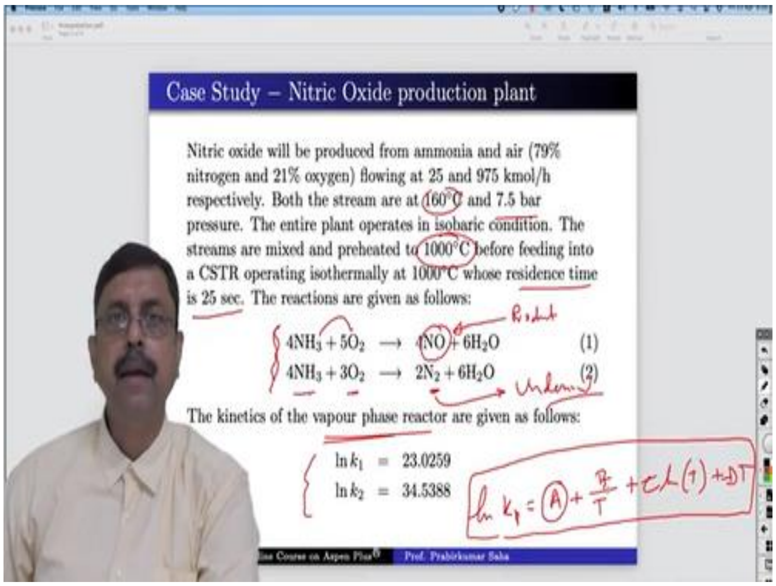

Welcome to the massive open online course on Aspen plus. In today's lecture we have come up with another interesting case study and it is on nitric oxide production plants. Now the nitric oxide will be produced from ammonia and air. Air means we assume that we have 79% of nitrogen and 21% of oxygen. If you use the air component in Aspen plus it will have many more things like it will have carbon dioxide, it will have some other components.

But in this problem, we will define air as a substance which has only 79% of nitrogen and 21% of oxygen, nothing else. So, this ammonia and air are flowing at 25 and 975 kmol/hr respectively and both these streams are at 160 ^{0}C and 7.5 bar pressure. So, the properties of the streams are defined over here. Now important information is given here, the entire plant operates in isobaric condition.

That means the pressure is the same throughout the system no matter which process equipment you use which block you use there will be no pressure drop. That means the pressure is at 7.5 bar so it will remain at 7.5 bar throughout. The streams are mixed and preheated to 1000 ^{0}C before feeding into a CSTR operating isothermally at 1000 ^{0}C whose residence time is 25 seconds. So, let us try to visualize the process flow diagram.

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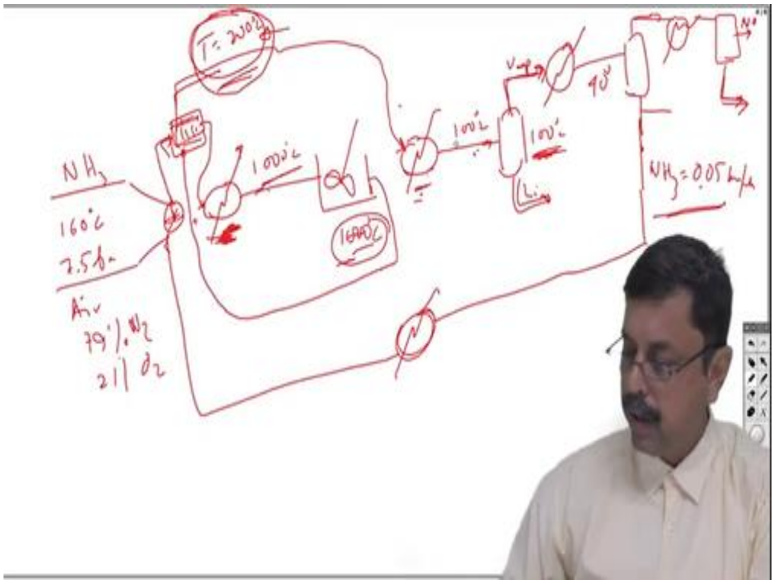

So, we will have two streams. So, this is ammonia and this is air. It will have 79% of nitrogen, 21% of oxygen. Both are at 160 ^{0}C and 7.5 bar pressure. So, they will be mixed in a mixture and they will be preheated to 1000 ^{0}C and then they will be put into a CSTR. And the CSTR also operates at 1000 ^{0}C. So, this is the flow diagram. Now the residence time of the CSTR is 25 seconds.

The reactions are given as these two. That means the ammonia reacts with oxygen and produces nitric oxide and this is our product. But it reacts with oxygen with a different stoichiometric ratio and produces nitrogen and this is an undesired product. But we cannot help it. These two reactions always occur together. As we know that the temperatures and pressure are very high, temperature is 1000 ^{0}C and pressure is 7.5 bar.

So, the entire reactor will work in the vapour phase. So, it is a vapour phase reactor. The kinetics of the vapour phase reactors are given in this fashion. Actually, the kinetics as you might understand in Aspen plus it is given as $\ln k_p = A + \frac{B}{T} + C\ln(T) + DT$ and then D into T. So, this is the complete equation of the kinetics. But in this particular equation B, C and D are 0. So, only a single constant term A remains.

So, that is the reason we find the reaction kinetics is of this nature. So, reaction kinetics are given for CSTR.

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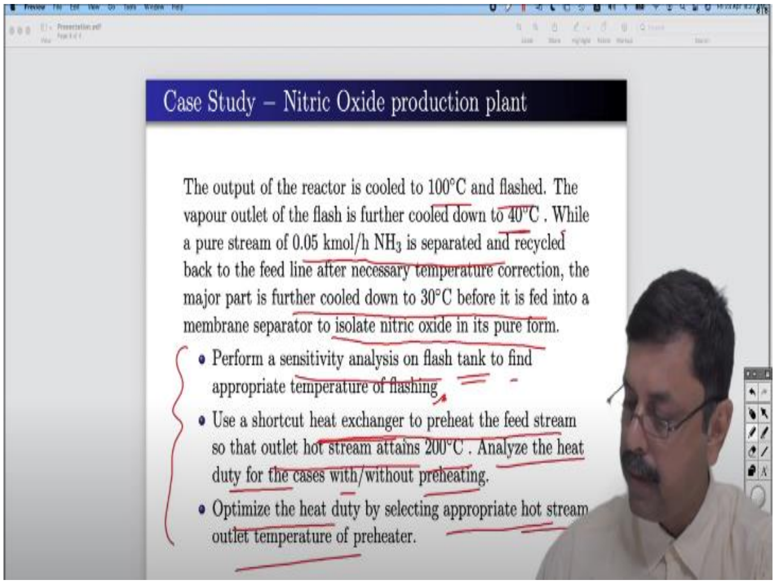

Now the output of the reactor is cooled to 100 ^{0}C and flashed. So, we have this one. We will use a cooler which will be cooled to 100 ^{0}C and then it will be flashed. We will have a liquid outlet and a vapour outlet of the flash. The vapour outlet of the flash is further cooled to 40 ^{0}C. So, this has to be cooled to 40 ^{0}C because it is operating at 100 ^{0}C.

So, it will be cooled to 40 ^{0}C and then a pure stream of 0.05 kmol/hr ammonia is separated and recycled back to the feed line after necessary temperature correction. So, there we have a recycle stream. It is defined as there is a separator and in this separator one stream. Here we have an ammonia flow rate of 0.05 kmol/hr. So, we will use a separator, simple separator.

It may be a membrane separator or something else and we will take out this much ammonia and this we will recycle but obviously before a temperature correction because it will be at maybe 40 ^{0}C or so. But here it will mix with 160-^{0}C feed. So, we have to have a heater over here and then it will go to another heater where it will be raised to 1000 ^{0}C before it is fed into the reactor. So, this is the recycle loop that we have to use.

And then the major part is further cooled down to 30 ^{0}C before it is fed into a membrane separator to isolate nitric oxide in its pure form. That means this is the major part which will be further cooled and then it will be passed through another separator where pure nitric oxide will be taken out and the rest will be purged. This is the total flow diagram. Now we have to do these three tasks.

What are they? First, we have to perform a sensitivity analysis on the flash tank to find the appropriate temperature of flashing. Right now, we are flashing at 100 ^{0}C because it is entering at 100 ^{0}C. But we should not be very particular about this temperature. We have to do some sensitivity analysis on this temperature and see the component profiles of vapour and liquid so, that we can judiciously fix the temperature of the flash.

And then we will use a shortcut heat exchanger to preheat the feed stream so that the outlet hot stream attains 200 ^{0}C. So, let us understand it better. Here this is an exothermic reaction and the reactor output is coming out at 1000 ^{0}C and we are cooling it down to 100 ^{0}C. So, here we are heating it to 1000 ^{0}C and here we are using a cooler to cool it down to 100 ^{0}C.

So, why not use the heated liquid over here to heat up or preheat this stream so that the heat duty on this heater is minimized because anyway we have to cool down this stream. So, maybe we can cut this stream. In place of that we will use the heat exchanger, we will pass this stream to this and then we will have a connection like this. And we will also take out this outlet stream from here; use it to preheat that stream and outlet of the stream we will attach to the cooler.

Then it will always be at a lesser temperature, less than 1000 ^{0}C. So, not only this heater but the heat duty of this cooler will also be reduced. So, that particular operation we will do. And we shall use a shortcut heat exchanger because already we have learned how to design a heat exchanger in detail in an earlier case study. So, we will not repeat them over here. So, we will stop at shortcut heat exchangers only.

But we will analyse the heat duty for the cases with or without preheating. That means we shall record the heat duty before we use the preheater and then we will see the heat duty when we use the preheater and check how much reduction of the heat duty that we could do by using a preheater. And lastly, we have to optimize the heat duty by selecting the appropriate hot stream outlet of the preheat.

For the shortcut heat exchanger method, we will set a parameter over here and the parameter is 200 ^{0}C. So, we will fix the outlet temperature to 200 ^{0}C. So, that is our condition. Now we may not fix it at 200 ^{0}C. We can do an optimization this may be a variable to define and the total of heat duty of this, this and this may be the objective function which we need to optimize and fix the temperature accordingly.

So, that optimization we have to do. Basically, we have to find out the temperature of the hot stream outlet for which the heat duty of this, this, this and this all of them added should be minimum that we have to find out. So, let us go to the Aspen plus simulation window and here we have to add up the components.

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First is obviously ammonia and then air that means we have to add nitrogen and oxygen. And then we will produce nitric oxide and we shall produce some water also, because if you remember the equation, in the equation we also have water. So, we can write H_2O and then the property method. The best property method for this case is NRTL, non-random two liquids. But we will also use the Redling Kwong equation of state with Henry's law.

Press next, run. It is done. Then go to the simulation window. Now we shall do the simulation part by part. So, first let us do it with a mixer, heater and reactor. So, based on the output of the reactor we will take the decision on this and this. So, let us take a mixer first. So, let us use this icon for a change and then we shall have a heater and then we shall have a reactor. And we will have a connection. So, this is one input, this may be ammonia and this may be air.

Let us connect this to the heater. This will be connected to the reactor and finally this is the output of the reactor. We have to rename them. Let us rename it as a mixer, let us rename it as heater 1, let us rename it as CSTR. This one we will write as ammonia, this one we will write as air, this one we will write as feed, this one will be reactor in, this is reactor out. So, first we have to define the feeds.

So, ammonia will be let us, check once again. It is 25 kmol/hr and 975 kmol/hr of ammonia and air is 79-21 oxygen and the temperature and pressure are 160 and 7.5 bar. So, we key in 1 that information, 160 ^{0}C 7.5 bar and 25 kmol/hr. This ammonia stream and air stream this is also 160 ^{0}C 7.5 bar and 975 kmol/hr with a mole fraction of 0.79 of nitrogen and 0.21 of oxygen.

So, ammonia and air have been fixed. Then we have to heat this up to 1000 ^{0}s C. That is the reactor temperature and obviously the entire system is isobaric. So, there will be no pressure drop anywhere. So, we will say pressure drop 0 and then we have to check the CSTR. Here the pressure drop is 0, isothermal reactor at thousand ^{0}C and we will have residence time.

Just check the residence time it is only 25 seconds. So, it is 25 seconds and then we have to fix the kinetics. Now here in kinetics we have to create a new reaction set which is of general type and set the reaction first. So, this is the new reaction. Give a reaction name. Before that it is an equilibrium reaction; so, set it as an equilibrium type, say RX1 is a component. First reaction is ammonia reacting with oxygen.

So, ammonia reacts with oxygen. In fact, both of the reaction's ammonia react with oxygen. Only in one case it produces nitric oxide and water. In the other case it will be nitrogen and water. For the first case our coefficients are 4 and 5 and 4 and 6. So, it will be 4, 5. Actually, it is a - 4, - 5 then it will be 4 and 6, - 4, - 5 because they are reactants. So, let us close it and create a new equation once again with equilibrium type. It is RX2.

Here also ammonia reacts with oxygen to produce this time it will produce nitrogen and water. Let us see the coefficients. Here it is 4, 3 and 2, 6. So, it is - 4, - 3, 2 and 6. Now we have to set the equilibrium. For the first reaction obviously, it will be a vapour phase reaction and it will work at 1000 ^{0}C and we will compute it from the built-in equation that is

$$\ln k_{eq} = A + \frac{B}{T} + C\ln(T) + DT\ .$$

Now in this case B, C and D are 0. We have only A. So, in the first reaction we have A = 23.0259. So, we write 23.0259 and in the second reaction this will also be a vapour phase reaction with a temperature approaching 1000 ^{0}C . Compute k equilibrium. In this case we will have ln k2 = 34.5388. So, we have got the expressions. So, the reaction kinetics is set already R1 we have defined. Now the system is ready to run.

So, let us run the system and see what happens. Yes, so it is run. Let us see the temperature and molar flow rate. Now there is no point in seeing the pressure because pressure is always 7.5 bar. If you check the pressure, it is actually not 8. We have to increase the number of digits of the decimal. So, once we do that, we will find it is 7.5 bars everywhere. So, let us not take this unnecessary, it will create clutter.

So, we have a temperature of 160 and a flow rate of 25975. Here it is entering at 1000 kmol/hr and exiting at 1006 kmol/hr and this extra six moles have been obtained because of the reaction. Anyway, we are at 1000 ^{0}C. But we have to reduce it down to 100 ^{0}C and then flash. So, we will use another exchanger. So, this is our cooler and then we will use a flash. So, let us rename them first.

So, this is cooler 1 and this is flash. I think we will have only one flash. So, there is no point in writing flash 1, flash 2. Now this we have to connect to this. Material stream is connected over here. This is our vapour phase and this is the liquid phase. So, we again rename them as flash in. This is flash vapour; this is flash liquid. And we have to set the temperature. So, let us set the temperature at 100 ^{0}C and 0 bar pressure for the heater or say cooler.

This is cooler actually. It is cooling the liquid from 1000 ^{0}C to 100 ^{0}C and flash it also operates at 100 ^{0}C with 0 pressure drop. Now let us run the process. It ran so quickly and we got everything over there. There is nothing in the liquid phase. So, perhaps we should not flash it at 100 ^{0}C. Let us reduce the temperature. So, we shall use 40 ^{0}C, run it.

Now we have got some material over here. Now let us check the stream results at the flash. So, we will have 769 almost 770 kilomole per hour of nitrogen and 173 kmol/hr of oxygen and rest nitric oxide and water. And we have very little amount of nitric oxide over there. So, entire nitric oxide they are going through the vapour phase. So, we have so much unreacted ammonia from here.

And we have got a lot of nitrogen because anywhere some amount of nitrogen was coming through the feed only and by breaking the ammonia, we are again producing nitrogen through the second reaction. So, obviously we cannot help. Nitrogen percentage will be very very high. Now obviously if you see the mole fraction. This is the mole fraction and if you just compare it with the reactor out and reactor in.

Let us see this is reactor in and this is reactor out 25 kmol/hr ammonia and in the reactor out we have only this much. So, almost the entire ammonia has reacted. The nitrogen amount is same. Here we find that not much nitrogen is being produced and then oxygen has reduced, earlier there was no you know. Now we have got this much of NO and this much of water. This is about reaction out. Now let us compare the FVAP.

So, in MVAP we have almost all the amount of nitrogen, oxygen and nitric oxide and also unreacted ammonia also. They are going through MVAP and if liquid is dominated by only water and that is understandable. Because all of them at 40-^{0}C ammonia, nitrogen oxygen and nitric oxide all of them will be vapour. But water will be in the liquid phase. So, you will definitely get most of the water to be going through the liquid stream.

Now let us check the diagram once again. The vapour phase will be further cooled to 40 ^{0}C. Now here we do not need to cool down because already we are at 40 ^{0}C. So, let us remove this one. At least at this moment we do not need this or we may need later when we change the flash temperature away from 40 ^{0}. So, let us use it. At this moment there will be heat duty of 0.

So, we will have an exchanger at this moment there is no need. But we just keep a separator. So, here this will be reconnected to the destination FVAP and then this will be connected to this one. And one outlet of the separator and this is the second outlet of the separator. So, let us rename. This is we do not know whether it is heater or cooler because it depends upon the temperature of outlet.

So, in future if we find the temperature of flash is higher than 40 ^{0}C then it will be used as a cooler. Else it will be used as a heater. So, write it as HC, so, neither heater nor cooler. Let us rename it as sep1 in. We will have two separators. So, we will write sep1 and then this one is sep1 VAP and sep1. Actually, both of them will be vapour phase only because there is no vapour and liquid over here.

One more thing is that we check the problem statement while a pure stream of 0.05 kmol/hr of ammonia is separated and recycled back to the feed line after necessary temperature correction. The major part is further cooled down to 30 ^{0}s C before it is fed into a membrane separator to isolate nitric oxide in its pure form. So, we will have this one as ammonia recycle.

This is 0.05 kmol/hr of ammonia and this one is the rest which will again further cool down to 30 ^{0}C. So, here it will be at 40 ^{0}, here it will be at 30 ^{0} and then we will use another separator which will separate nitric oxide in its pure form. So, we shall use a cooler and let us write it as cool 2 because we have already used a cooler one over here and this one is sep2. So, let us connect this.

Reconnect destination over here and then this one with this and this one this and this one this. Let us bring it down. Now again we have to rename them. First rename it as sep1 out or c2 out. This should be c2 out and this one we will write pure NO. Because the stream will have 100% purity with NO, nothing else and here we will say rest. So, all the other things will be purged through this. Now let us fix this.

This one will be temperature 40 ^{0}C 0 bar pressure drop. And this one will have ammonia recycle. So, we will say the ammonia recycle stream will have a flow rate of 0.05 kmol/hr. So, that is what it is said over here. You can check while a pure stream of 0.05 kmol/hr ammonia is separated and recycled back. So, basically this is the recycle line that we have to attach over here.

And then cooler 2, obviously, the cooler 2 will reduce the outlet to 30 ^{0}C and no pressure drop. And this separator we have to send pure NO at the top. So, we will have NO split fraction 1 and rest will be 0 and in sep1 also we have to make all others 0 otherwise there will be a problem. So, here it is 0 and all others we have to make 0. Now let us not connect the recycle stream.

Now we shall run the system without recycle once, check the result and then we shall run with recycle and see whether we have got some changes. So, let us run, yes. So, let us see the purity of NO. It is 25 kilo moles per hour. Now let us increase the number of digits after the decimal point. So, 24.8471 of nitric oxide is being produced. Here we have 27.7425 kmol/hr but out of which we have only water, all others are less.

Here also out of 953 there is almost no ammonia. Nitrogen and oxygen are having the bigger share water and ammonia are not that much. But this is pure NO you can check. We have given a membrane separator in that fashion. So, it is completely pure NO. Now we will check whether by recycling we can increase it. So, let us freeze it first with this component and recycle. So, for recycle obviously we have to, this is at 40 ^{0}C now we have to increase it up to 160.

For that we have to do a certain temperature connection. So, we will use the heater over here. Now let us connect this. So, this one reconnects the stream to its destination. This end and this one connects to this edge. So, we write it as a heater 2 and this is H2 out. And heater 2 will hit the stream from 40 ^{0}C to 160 ^{0}C with 0 pressure drop. This is a special kind of system that we are working with.

Here the entire system is operating at the same pressure and we do not have to bother about the pressure changes. Everywhere we keep the pressure drop to be 0 and we do not have to check the pressures anywhere. Only we have to do temperature correction. Anyway, so the recycle is connected now let us run once again and please check it. It is now 24.8471. Now if we run let us check whether the value changes.

Yes, it has increased. So, earlier it was 24.8471. Now it is 24.8963. So, obviously the amount of production of nitric oxide has increased. Now we have to do one task over here which we should have done before but even now it is not late. The task is first we have to perform a sensitivity analysis on the tank to find appropriate temperature of flashing. So, right now we are flashing at 40 ^{0}C. Now let us check with a wider temperature range.

So, for sensitivity analysis we have to go to the sensitivity analysis tool, press new and then we will vary the block variable. Which block? It is flash and the variable is the temperature and we shall begin at 0 and end at 100 for the entire range. Let us see we can give an increment of 1 ^{0}C. So, basically, we will have at 0, at 1, at 2, at 3 and so on. Now we will define three things.

One is purity of NO or flow rate of NO and also the flow rate of water all in the vapour line. I will explain why I am choosing this. So, what is the purity of NO? This is a stream variable of mole fraction in nature of the stream FVAP the component NO. Flow same thing but it is mole flow. Stream is MVAP again and component NO. And finally, water flow so, again it will be a molar flow of stream MVAP the component water.

And we will tabulate all of them. Press run. Now just check the results. So, from temperature 0 ^{0}C to 100 ^{0}C we have the entire range. Let us check the results curve. So, temperature versus all of them in y axis, press ok. Now after 67 ^{0}C the purity of nitric oxide goes to minimum. Although the flow rate is maximum but purity is minimum.

So, you definitely would not like to go with this purity but again check the water flow rate. As the temperature increases the flow rate of water increases also, when the temperature is lower the flow rate of water is less. Purity of NO is high but we have to compromise with the flow rate of NO which will be lower. But we can come with a trade somewhere here at this point where we will have reasonably higher flow rate of NO, reasonably higher purity of NO and comparatively less amount of water.

Because when you have a high flow rate of water then some of these gases will mix in water and a lot of acidic stuff may be produced which you probably want to avoid. So, maybe a temperature of this range is ideal for your operation where your flow rate of nitric oxide is reasonably high and the purity of nitric oxide will also be reasonably high. There is a trade-off and the water flow rate are also reasonably low.

So, let us operate the flash somewhere around 35 ^{0}C. So, right now we are operating the flash at 40 ^{0}C rather we shall operate it at 35 ^{0}C. So, it is 35 ^{0}s C. So, it will be regarded as a heater. So, let us run it. It has converged and at this moment there is no point in working with the sensitivity analysis. We just make it inactive. Let us run it once again without sensitivity analysis. Yes, it has run very fast.

Now this is done. Next, we have to use a shortcut heat exchanger to preheat the feed stream so that the outlet hot stream attains 200 ^{0}C and we have to analyse the heat duty for cases with and without preheating. So, at this moment let us see what is the heat duty. Now this is a case without preheating. Right now, we are not using any preheating. So, let us check the heat duty and we have to calculate these figures.

We have to calculate this one, this one and this one. So, once we use a preheater these three things will change. So, let us calculate them. We have a simple calculator where we have to add these numbers. So, if you add this plus this plus this you will obtain 4136465. This much of heat duty Q total is this, this much cal/sec. Now we have to check whether we can reduce this total heat duty by using an appropriate preheater.

For that we have to first keep these two things away, so, that we can have some extra room for the preheater. Now let us use a heat exchanger over here. Now in this case this is the cold fluid. So, we reconnect the stream at this destination and this outlet will come to this one. Now we will keep this thing over here. That will look better reroute this stream and then this outlet we shall reconnect with this one and this outlet will reconnect with this one.

So, this is the total figure after using the preheater. So, this is the feed it is entering into the preheater which is a heat exchanger and this is hot out and this is actually hot in. Let us rename it as hot in and this is feed. Actually, we can write it as cold in and this one is cold out. So, we have to define the preheater condition. Now it is shortcut but some extra information is given that outlet hot stream attains 200 ^{0}C.

So, while fixing the preheat specification we have to use shortcut counter current. And hot stream outlet temperature is 200 ^{0}C. So, that we have fixed it now. Now let us run at this condition. So, again it has converged and we are happy. As expected, the outlet temperature is 200 ^{0}C. Earlier in this case the heater duty was so much 1821968. But now as we are using a preheater this has come down to five digits.

Obviously, a new heat duty over here comes up. What is the total amount now? Let us check once again. So, this one is this plus this plus this plus this. So, the total figure comes 2397748. So, this is the Q total. So, the new figure is 57% of this. So, almost 43% of the reduction of the value has come up by using a preheater. So, we have done this we have analysed the heat duty for the cases with and without preheating.

And with preheating we have reduced the heat duty by 43%. Now the third and last task we have that is optimize the heat duty by selecting appropriate hot stream outlet temperature. Now this 200-^{0}C is arbitrary. It has been studied in the problem statement so we have taken. But we have to check what temperature we should use so that the heat duty is minimized. For that let us go to model analysis tool and press this optimization.

Open a new optimization routine and there we have to define a new variable and the variable name is q preheat which is a block variable. Which block? The preheater. Which variable? It is heat exchanger heat duty. Then we will say QH1. Again, it will be a block variable which is of block H1 and the variable is heat duty. Similarly, we can copy this and paste this one we shall write for c1 and CSTR. So, we rename it as QC1 and this is for c1.

All other things are the same and we shall paste once again over here that we write it as CSTR and this is for CSTR. So, we have taken up the heat duty for all four things, preheater, heater, cooler and CSTR. Just check. We have taken it for preheater, heater, CSTR and cooler all of them. So, what is our objective? So, we have to minimize Q1 or Q preheat. But you can check it from here variable list. So, QPRE + QH1 + QC1 + Q CSTR. So, all of them we attach.

What should I vary? We will vary the new variable which is again a block variable. It is a block variable. Which block? It is the preheater and we shall change the hot stream outlet temperature. So, we have to look for it. This one should be specified outlet temperature of the hot stream. So, just click it and we do not know what should be the value. But we can give say 130 ^{0}C to 270 ^{0}C.

So, actually right now we are operating at 200 ^{0}C. Let us take 70 ^{0}s down and 70 ^{0}s up and let us see where actually we get the minimum. Now one thing is there you have a negative sign with CSTR and c1. So, you cannot use plus sign over here. Then they will be added up with negative sign. So, you have to go to the one input an objective constraint. Here you have to give minus and here also you have to give minus.

So, that the negative sign gets positive over there. And there you can run the simulation. Now we have got the result. We have got it at 161.482 ^{0}C. So, what the optimization routine says is that if you operate your preheater with an outlet hot stream temperature of 161.482 then you will get the total heat duty. It will be 2320541 cal\sec. So, this one if you compare it with the original figure, we have reduced 4% from this figure. So, this is even 4% less than the previous figure.

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So, we completed the last task also that is optimization of the heat duty by selecting appropriate hot stream outlet temperature of the preheater. So, with this we come to the end of this case study of nitric oxide production plant and we shall come back with another case study in the next lecture. Till then thank you and goodbye.