Aspen Plus Simulation Software - a Basic Course for Beginners

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Lecture - 07
Using Model Pallete – Reactors

Welcome to the massive open online course on Aspen plus.

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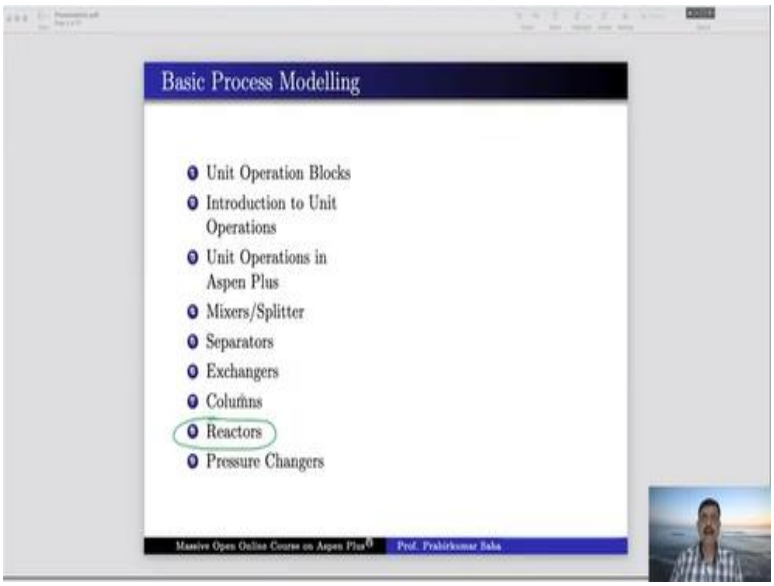

In today's lecture, we shall learn about the simulation process of reactor models in Aspen plus.

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If you look at the simulation window of Aspen plus, you will find the following blocks for the reactors. These are the blocks you will find RStoic, RYield, REquil, RGibbs, RCSTR, RPlug, and RBatch. These blocks can be subdivided into three main categories.

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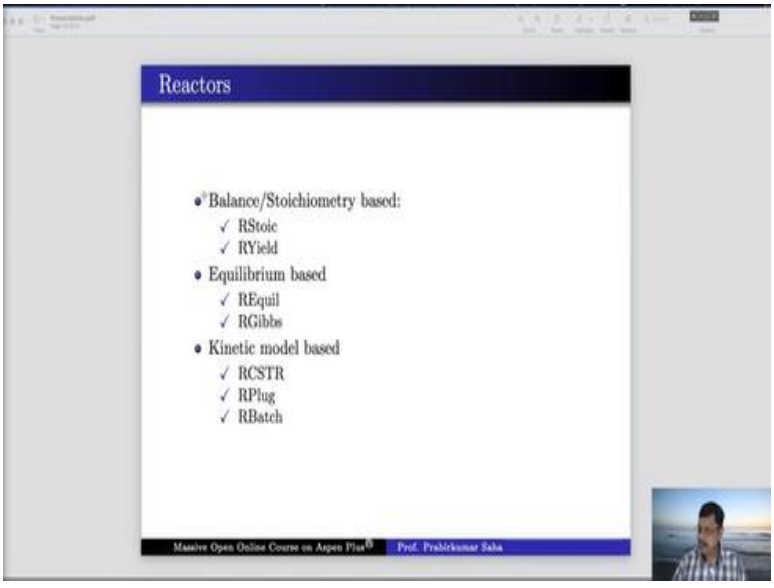

RStoic and RYield, come under the category of balance and stoichiometric based reactors. Equilibrium-based category they have REquil and RGibbs model blocks as given over here, and these three are common reactors that we all know RCSTR that is continuous star tank reactor. This is plug flow reactor and this is batch reactor. And these three they come under the kinetic model-based category. So, we will learn them one by one.

First, we will learn this balanced or stoichiometric category. Then we will learn equilibrium-based category and then finally we will learn kinetic model-based category.

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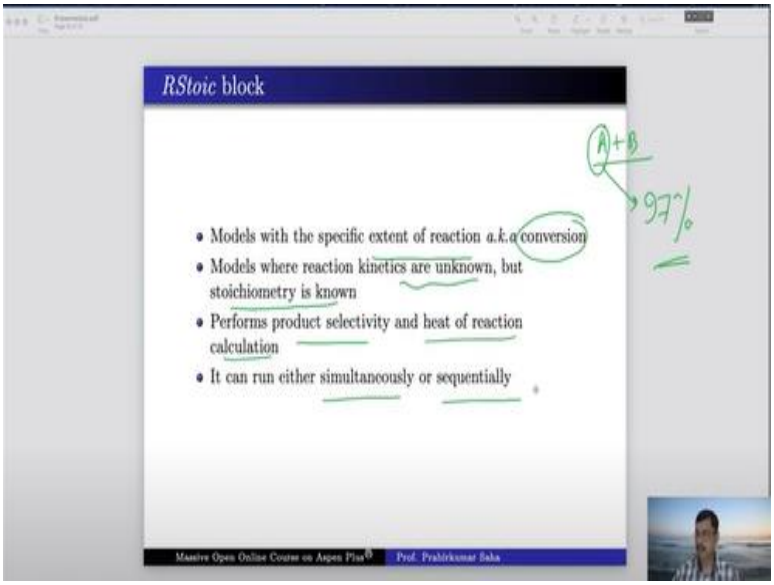

First is RStoic block. This block model with a specific extent of reaction is also known as conversion. So, suppose you are having a reactant A and B, and if you say that this reactant A will have a conversion of 97%, then that information can be given into this RStoic block. Then models, where reaction kinetics are unknown but stoichiometric, is known. It performs the product selectivity and heat of reaction calculation, and it can either run simultaneously or sequentially.

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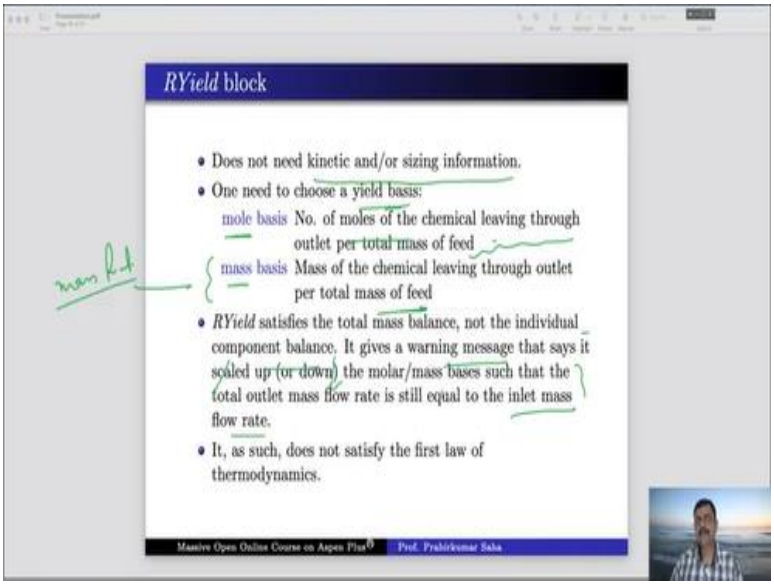

On the other hand, RYield block does not need any kinetic or sizing information. But it works on some yield basis. The yield basis can be either molar or mass that means the number of moles of chemicals living through the outlet per total mass of feed. And mass basis it is mass of the chemical leaving through outlet per total mass of the feed. You can say mass fraction. RYield satisfies the total mass balance, not the individual component value.

Sometimes it gives a warning message that says it has scaled up or scaled down the molar or mass basis such that the total outlet mass flow rate is still equal to the inlet mass flow rate. We will learn it better when we do the simulation. And finally, it as such does not satisfy the first law of thermodynamics. So, it is always an approximation sort.

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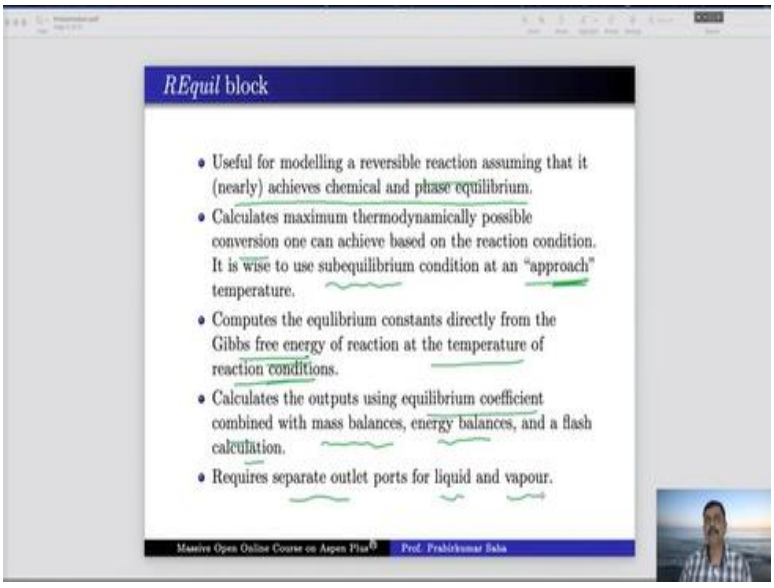

REquil block is useful for modelling a reversible reaction assuming that it nearly achieves chemical and phase equilibrium. It calculates the maximum thermodynamically possible conversion one can achieve based on the reaction condition. So, it is wise to use sub equilibrium conditions at an approach temperature. We learn about the approach temperature later. It computes the equilibrium constants directly from the Gibbs free energy of the reaction at the temperature of the reaction condition.

And it calculates the outputs using equilibrium coefficient combined with mass balances, energy balances, and flash calculation. And most importantly, it requires separate outlet ports for liquid

and vapour. For other reactors, there is no separate port for vapour and liquid. But in this block, you have to have separate ports.

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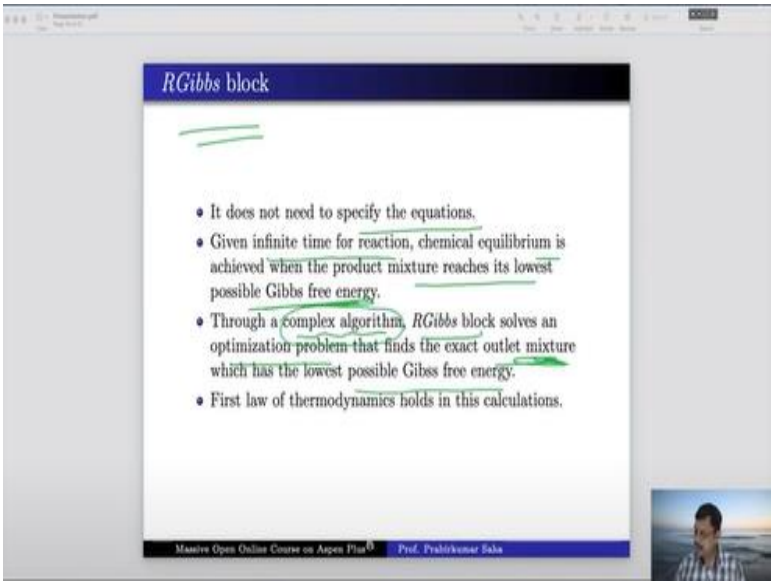

And then comes RGibbs block. It does not need to specify the equations. Given infinite time for a reaction, the chemical equilibrium is achieved when the product mixture reaches its lowest possible Gibbs free energy. In other words, this block calculates the maximum extent of conversion that a reaction can achieve. RGibbs block solves an optimization problem through a complex algorithm that finds the exact outlet mixture with the lowest possible Gibbs free energy. And definitely, the first law of thermodynamic holds in this calculation.

Without that, we cannot get the minimum Gibbs free energy calculation. So, we shall learn about these four blocks, which I have talked about RGibbs, RYield, REquil, and RStoic using this small exercise with water gas shift reaction.

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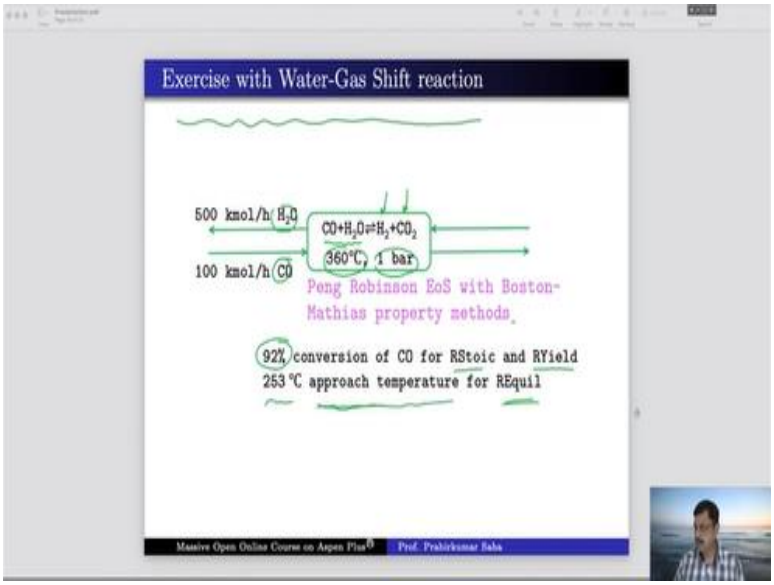

As we all know, a water gas shift reaction is about reacting carbon monoxide with water at 360 degrees centigrade and atmospheric pressure to achieve hydrogen and carbon dioxide. The flow rate of carbon monoxide and water is given, and we shall use the Peng Robinson equation of state with Boston-Mathias property methods. For RStoic and RYield, we need this information 92% of conversion of carbon monoxide.

Whereas an approximate approach temperature has been given for our equilibrium which is 253 °C. So, we need this information for calculation. So, let us see how these blocks can be used for calculation in Aspen plus simulation window. So, for that we need to specify the components.

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So, our components are carbon monoxide, carbon dioxide, water, and hydrogen. Press Next, we have to use Peng Robinson equation of state with Boston-Mathias property methods. So, we get it here paying revenues and equation of state with Boston-Mathias modification. So, you press next and run so property estimation is complete, go to simulation window. We directly go to the flowsheet, so in the reactor, first we bring RStoic.

This is a material stream and this is the product stream we name feed and here we name PStoic that is product from RStoic block. Press next, we have to give the temperature of feed. So, this is 360 °C and 1 bar pressure and we have 500 kmol/hr water and 100 kmol/hr carbon monoxide. So,

press next. Now it is asking for the inputs for RStoic model. So, temperature and pressure we have to specify 360 °C and 1 bar and the reaction.

So, the reaction we have to press 'New' and here component CO carbon monoxide reacts with water to form carbon dioxide and hydrogen. So, coefficient - 1, - 1 because they are reactants and these are products. And fractional conversion has to be given, which is 92% conversion of CO. So, 0.92 of CO. Press next, now it is ready to run. So, run the result is available, go to stream results. So, here you can see in the feed we had 100 kmol/hr of carbon monoxide.

But in the product of stoichiometric reactor, we have only 8, 8 kmol/hr carbon monoxide. So, 92 kmol per carbon monoxide has been converted into carbon dioxide. And similarly due to stoichiometric equivalence 92 kmol/hr of hydrogen has been produced. Now let us see how RYield works, for that let us go to main flow sheet once again bring in RYield over here.

We shall use the same feed over here. So, let us first use a manipulator here is a duplicator. We shall connect this line with the duplicator and then do the material stream connection between the duplicator and the reactors. And we have to rename it let us rename it as PYield. Now press next feed has already been defined. So, is the RStoic, so, RYield has to be defined here. So, temperature is same 360 °C and 1 bar pressure.

The yield has to be specified component yields. Now here we have to check whether we want to give it on molar basis or mass basis. In my opinion, at least for this problem, watching mass basis is better because we already know the result in the RStoic model. Here, if you see mass fraction, then you will find that it is 0.0189761 so, 0.0189761. Carbon dioxide again mass basis water, mass basis and hydrogen again mass basis.

So, carbon dioxide will have 0.342875, water 0.622443 and finally hydrogen 0.0157055. So, all the component yields are specified. So, we can run the simulation, now we can check the result once again. So, we can place PYield side by side with PStoic to compare the result. Here we can find that there is slight changes in the values. Here you will find certain warning messages that is a sign of this nature.

So, we can further explore what they mean. So, for that, you go to the results and see the status. Here, specified yields have been normalized by a factor of this to maintain an overall material balance. So, it is as good as the error message or warning message that I was specifying some time back. It scales up or scales down by doing certain normalization to make the inlet mass flow rate equal to outlet mass flow rate.

So, RYield again it is some kind of approximation and we have to accept this result in this manner. Anyway so, let us keep our result in this fashion only, we will analyse it later. Now let us see how the R equilibrium block works. For that bring in the R equilibrium connect the material streams. And here you can see that we have to give two outlets. One is vapour another is liquid because that is the norm for any equilibrium reactor.

Now let us write it as VEquil and let us write it as LEquil. Press next, we have to give the temperature-pressure condition which are same as before. Then we have to specify the reaction. So, the reaction reactants are CO and water; products are carbon monoxide. And hydrogen coefficients for reactants are - 1 and - 1, whereas coefficients for products are 1 and 1. Here we have to determine the products by specifying the temperature approach to equilibrium.

Here one data has been given 253 °C approach temperature for R equilibrium. So, 253 °C if we provide as an approach temperature and run let us see what happens in the results block. So, the results are available. Let us know what the results are. Here we write VEquil and LEquil. Now here you can see one thing that is in LEquil everything is 0. So, there is obvious because at 360 °C you will not find any liquid because you have CO, CO_2, water and H_2.

So, at 360 °C none of them can be in liquid phase. So, there will not be any liquid over there; everything will go as a vapour. So, that is obvious. Now in vapour phase if we see the mole fraction of carbon dioxide is 0.159256, whereas with a stoichiometric reactor it is 0.153333. The mass fraction of carbon dioxide calculated by the REquil block is 0.342031, whereas calculated by stoichiometric reactor it is 0.342875 and that is using 253 °C temperature approach.

Now let us try to see what happens if we increase the temperature approach or if we decrease the temperature. For that let us change the data in input block. So, we change it to 260 °C. Now at this moment it is 0.342031. If we run and see what happens, so it decreases at if we make a higher temperature then the value decreases and if we take a lower temperature obviously it will increase.

So, if we take instead of 253 °C if we take 240°C then definitely this will increase, it has increased. So, we want to know at which temperature approach the value of CO_2 will be exactly 0.342875. For that we can do certain sensitivity analysis. Although I will teach the sensitivity analysis in some future lecture. But today for the example it is important to learn how to do it. So, for that we have to go to this model analysis tool and say sensitivity analysis.

So, press a 'New' enter id S 1 and then type a variable new. This is a block variable. So, we have to choose the block B 5 because that is the equilibrium block and the variable. Let us look for the variable what the variable is we have to say approach, temperature approach. Let us see what is this? This is the one temperature approach to equilibrium. So, DELT is the one which we are looking for.

Let us give an idea of one in degree centigrade and we start from 240 °C and end at 260 °C with an increment of 1 °C. Then define a variable say give a name of the variable say V 1 actually it is a stream variable which is mole fraction of stream VEquil and component say carbon monoxide. Go to tabulate and fill variables column number VA 1, let us run and see.

So, run results are there just go to results. So, you can see from 240 °C approach temperature, at 240 °C approach temperature it is 0.153768. So, if you see mole fraction it is 0.153768 at 240 °C and at 260 °C it is 0.152513. So, actually we want the value which is very close to 0.153333. So, which is the nearest value for 0.153333, it is 247 °C. So, let us redo this once again between 246.5 to 247.5 °C. So, go to input, so 246.5 to 247.5 °C, with an increment of say 0.01 °C and run it once again.

So, results are available so you can just go and see where exactly it matches. So, here you can see 246.98 °C, 246.99 °C at this temperature the mole fraction matches with stoichiometric reaction.

So, we can use either of them 246.98 ℃ or 246.99 ℃. So, let us use 246.985 ℃. So, go to block input reaction, edit it, give the temperature approach as 246.985 ℃. And run the simulation once again. Just go and check and this is the result you get.

It matches everything matches with RStoic. So, to achieve this amount of mole fraction in the product that is the temperature approach for equilibrium. Finally, RGibbs, so for that let us bring in RGibbs block over here. Connect the materials rename it to PGibbs, press next. Here we have several calculation options. We can ask for phase equilibrium and chemical equilibrium calculation.

We can ask for only phase equilibrium calculation or restrict the chemical equilibrium by specifying the temperature approach or specify duty and temperature and calculate the temperature approach. For this example, let us take the calculate phase equilibrium and chemical equilibrium option. Here, we have to specify the pressure and temperature once again and then everything seems to be specified. Just run the simulation and check the result PGibbs.

So, here you can see PGibbs have calculated the lowest point of Gibbs free energy. So, this is the maximum extent of reaction that can happen, like carbon dioxide cannot be produced more than this mole fraction. In other words, there cannot be more than 98.72% of conversion. At this conversion, the Gibbs free energy is lowest for this kind of reaction. Now, if we want to limit it up to 92%.

Then what is the Gibbs free energy up to that point? That also we can calculate from here. We have to choose a specified temperature approach or reaction extent and then choose 'restrict equilibrium'. And again, the temperature approach or molar extent for individual reaction. So, press 'New' press CO, water, CO_2, hydrogen, - 1, - 1, 1 and 1. And here you can write 92 kmol/hr or you can say temperature approach as it was said 246.985 ℃ that was the temperature approach we had given over there.

So, let us use this, now you can run the simulation and check the result and you can see the result with PGibbs. Here it is not going up to 98% calculation, it is up to 91.999% and actually 92% you

can say because you have restricted the equilibrium. Now we shall learn the last three reactors that is CSTR, plug flow reactor and batch.

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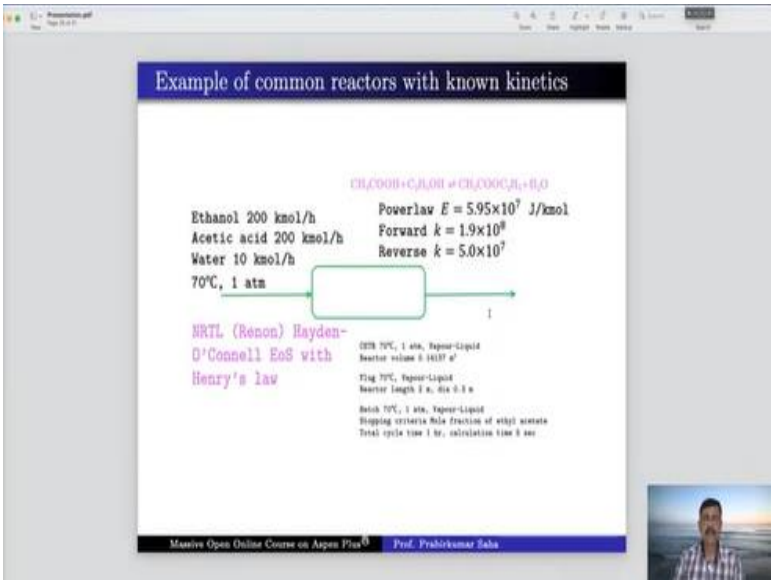

For that we open a new simulation block and we shall use this example of common reactors with known kinetics. In this reactor we have ethanol, acetic acid as a reactant and from them we produce ethyl acetate and water. The flow rate of the reactants and the temperature pressure conditions are given. And the reaction kinetics the K value and activation energy are given and we will use NRTL Renon Hayden O Connell EoS with Henry's law.

For CSTR plug flow reactor and batch reactor individual conditions are given. So, with this information we will see how these models can be used. So, the components are ethanol, acetic acid, water and ethyl acetate.

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So, we have ethanol, acetic acid, water and the product ethyl acetate. We have to find an ethyl acetate we have to select this one just rename it to eth acid. Next, we shall use NRTL Hayden O Connell equation of state with Henry's law. So, NRTL it is here Renon Hayden O Connell equation of state with Henry's law. Press next, run the properties are calculated, go to simulation block.

So, let us first take CSTR and the material streams and then rename them this is feed and this is PCSTR product CSTR. Press next the temperature and pressure condition it is 70 °C and 1 atm pressure. So, 70 °C and 1 atm ethanol and acetic acid 200 kmol/hr, water kmol/hr. So, it is 200 kilo mole per hour, 200 kilo mole per hour and 10 kmol/hr so this is the feed input go to Next. So, CSTR pressure again it is one atmosphere and temperature 70 °C, valid phases we have both vapour and liquid

.

The reactor volume is we have to write 0.14137 m^3, 0.14137 m^3. Now you may be curious to know what is the reason for giving such odd value in the reactor volume. For that we have to see the plug flow reactor. You may notice that the plug flow reactor the length is 2 m and diameter is 0.3 m. So, the volume of plug flow reactor should be

$$\frac{\pi}{4} \times 0.3^2 \times 2$$

So, if you calculate this will be equal to 0.14137. So, in order to compare the result, we wanted to keep the reactor volume same for both CSTR and plug flow reactor as well as batch reactor. Now we have to press the reaction kinetics we do not have any reaction kinetics available. Now we have to go to the reactions and define a new reaction over here. So, reaction id R 1 which is of power law type.

So, we have a power law equation with this. So, say stoichiometric ethanol reacts with acetic acid to produce ethyl acetate and water. The 0 coefficient should be -1 and -1 for them because they are reactant and their product so they are 1 exponent will be 1 and 1 for them and it will be 0 and 0 for them because they are product. Reaction type is kinetic. Now this is the forward reaction but we have reverse reaction also, this is both way.

So, we have to define the second reaction also where the component ethyl acetate will react with water to produce ethanol and acetic acid. So, here it is - 1, - 1 and this is 1 and 1, exponent 1 and this is exponent 0 because they are products. And as because they are kinetic reactions so we have to give the kinetic information over here. So, the K values for forward reaction is 1.9×10^8 and E value activation energy is 5.95×10^7 J/kmol.

So, this is for reaction number 1 and reaction number 2 again it is in reverse reaction it is $5x10^7$. And activation energy is same which is $5.95x10^7$ J/kmol. Now they are defined. So, the reactions are defined now we can go to the reactor setup and define this kinetics. Now R1 is available just select R 1 over here and run it. So, the run results are available, go to the stream results and see.

So, as it is equilibrium reaction so there is no change in moles and out of 200 kilo moles of ethanol 136 moles have been converted 73 moles remains for both ethanol and acetic acid. So, this is how the reaction took place. Now let us see how Plug flow reactor works in comparison with CSTR. So, bring in the block for plug flow reactor. For the same feed so here again, you have to use the duplicator, bring in the duplicator over here.

You have to manipulate with the feed line. So, just bring it over here and reconnect the material streams in this fashion. And we have to rename it as P Plug product of plug flow reactor. Press next so the specification for plug flow reactor is being asked. Here the reactor type it may be reacted with specified temperature or it may be adiabatic reactor or reactor with all those specifications that we can specify.

But for this particular reactor we will use reactor with specified temperature which is 70 °C as it is taken for CSTR. Now go to configuration we have to give the reactor dimension for plug flow reactor which is again we have done the calculation before 2 m and 0.3 m diameter. So, 2 meter and 30 cm diameter and the reactions are already defined before. So, just choose that reaction and your run is ready.

So, results are available again just go to the stream result of CSTR and add in the result for log flow reactor as well. So, unfortunately, we do not see any reaction to happen in the plug flow reactor as if the feed has entered and it has come out of the plug flow reactor without producing any water or ethyl acid. But that cannot happen we must have done some mistake. Let us go back to plug flow reactor and see what mistake we have done.

This is the mistake that we have done. The process stream we said vapour only. But at 70 °C, we cannot expect water or ethanol on them will be in vapour phase and react. So, we should write liquid only or vapour liquid. So, if we do not give vapour liquid then there will not be any reaction. So, we just run it once again with vapour liquid and check the result. Now you can find some product, 140 and 130 kmol/hr.

Now here you can find that the amount of ethyl acetate and water produced in plug flow reactor with 0.14137 $m^3$is more than that has been produced in CSTR. So, this results matches with our understanding with the theory of CSTR and plug flow. But for the same size of reactor for plug flow and CSTR, the conversion in plug flow is more than CSTR and that result is observed over here.

Now we come to the final reactor that we have for this lecture that is the batch reactor. And we have to connect this inlet and outlet, we have to specify it as PBatch. Now here you might be confused that it is a batch reactor but we are giving a continuous stream of material. Actually, in Aspen plus we do not have any input that can be batch in the strict sense. We have to define certain parameters in the batch reactor setup, which will make it a batch from the continuous stream.

Now let us see how we can make it batch. So, press Next so, we have to first specify the operating condition which is constant temperature at 70 °C and we will specify the reactor pressure which is 1 bar or 1 atmosphere, I think. And we have to give the reaction kinetics which has already been specified before and the stop criteria which is very important up to what point the batch reaction should be continued.

After that point we should stop the reaction that means that is the batch time. For that we can select the reactor, this is the location, variable type, mole fraction. Let us assume that we will stop the reaction when the mole fraction of ethyl acetate becomes 0.308018. So, 0.308018 that is the final point that we want to achieve for ethyl acetate. So, we will say mole fraction stop value 0.308018 of component ethyl acetate and approach from 0 that means initially it was at 0.

So, from below so 0 to 0.308018, it will go and calculate. Let us see this is the criteria number 1 and we have only one criteria, we do not see any other criteria. And then this is the operation times it is very important. This is the total cycle time in other words you can say it is a total batch time. So, if we give 1 hour then you can compare with the feed stream the feed stream is so many 410 kmol/hr.

So, if your batch cycle time is 1 hour then your batch charge is 200 kilo mole of ethanol, 200 kilo mole of acetic acid and 10 kilo mole of water that is your batch size. So, by specifying the total cycle time you are actually specifying the batch size and here you make it purely batch. And the maximum calculation time is again important because most of the reactions are very fast, at least this reaction is very fast.

From the experience we can see the reaction is over within a few seconds. So, we can say that we shall calculate only for 10 seconds with one second of interval in between them. So, the specifications are complete now we can run and see how the batch reaction runs. So, just go back to the stream results and add in the P batch and see it has stopped when the mole fraction of ethyl acetate is 0.3080, at this point it has stopped.

So, it is matching with the data of PCSTR stream. Now one more thing that you can see over there. Just go to the setup here you can bring in the composition reactor molar composition of ethyl acetate, press okay. So, this is the composition you get. Let us make it final calculation. So, instead of one second, we make it 0.1 seconds and run the simulation once again and see the plot. Now it is better.

Now convert the time from hour to seconds. So, you can see the reaction is almost complete within 2.15 seconds. And if you want to check the operation time it is 2.1501 seconds beyond that, the operation does not take place because by that time your preferred mole fraction of ethyl acetate is achieved and this is the total heat load in joules. And heat duty also you can calculate in kilowatt it is -1.22143 kilowatt.

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So, that is how you can do the simulation for reactor models in Aspen plus. So, we end our lecture at this point today. Thank you.