Aspen Plus Simulation Software – A Basic Course for Beginners

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Lecture-20
Introduction to the Course and Basic principles of Image Formation

Welcome to the massive open online course on aspen plus.

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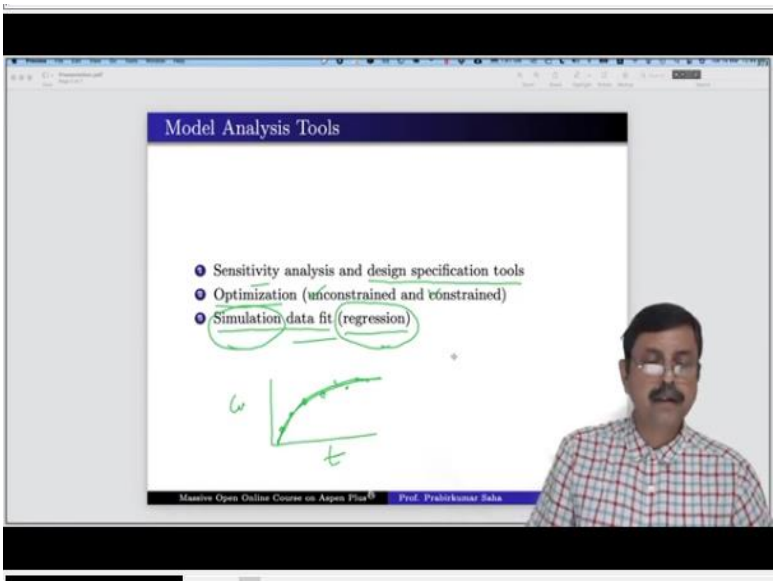

In today's lecture we shall discuss about the model analysis tools.

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We shall get this model analysis tools in the simulation window of aspen plus, it will be available over here. So, in this model analysis tools we will have the following things, the sensitivity, optimization, constraints and data fit. So, we will learn these things today.

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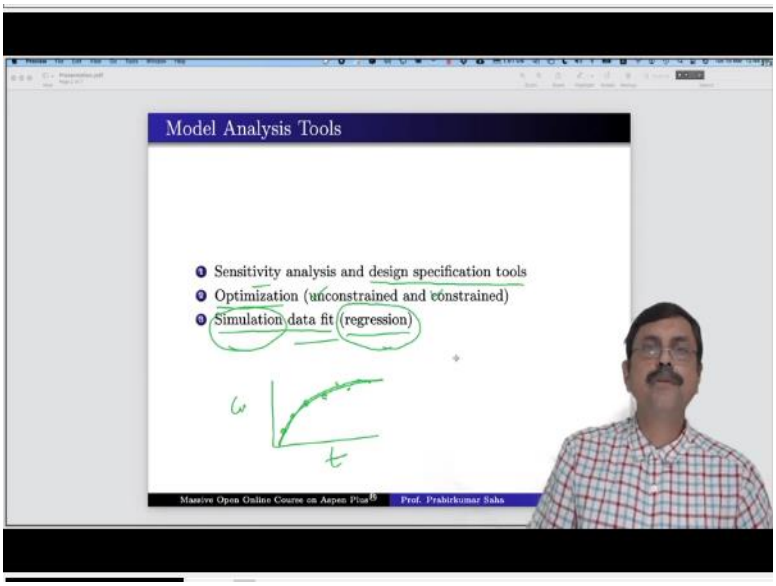

So, we have 3 major portions of today's lecture, the first one is sensitivity analysis and design specification tools. The second one is optimization; both unconstrained and constrained and finally the simulation data fit which is another way of saying regression. Now this regression we have already learned while we studied the property estimation and property methods. But here we shall learn the simulation data fit for simulation purpose.

That means suppose if we have a reactor data in batch reactor time versus concentration, so if our experimental data is something like this then we shall try to learn for what kind of reactor parameters our model reactor will follow the profile of experimental data. So, we shall learn one by one. Let us begin with the sensitivity analysis and design specification tools. And for each one of them we shall take an appropriate example and try to solve a problem so that we can learn it better.

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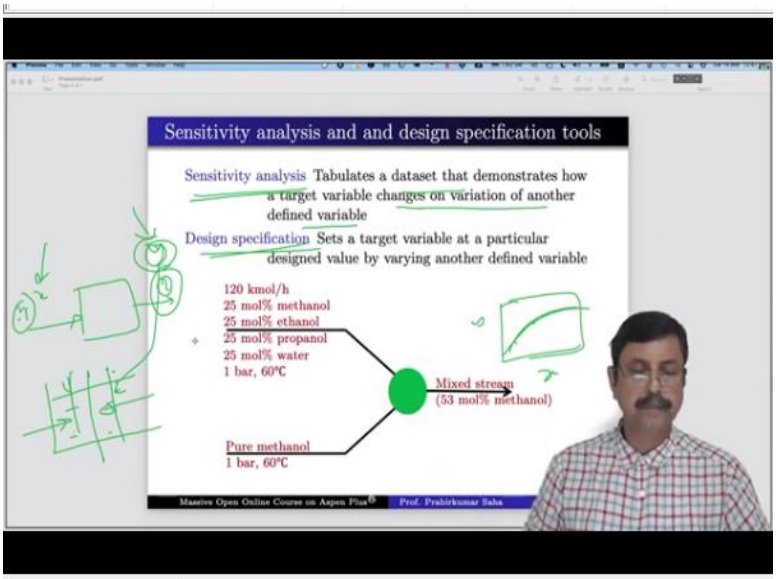

So, let us begin with the sensitivity analysis and design specification tools. Now both of them are done in a similar way, but there are slight differences which we shall have to understand first. The sensitivity analysis tabulates a data set that demonstrates how a target variable changes on variation of another defined variable. Suppose in a simulation you find that if you change a certain input variable then this particular output changes then our sensitivity analysis will tell you what will be the profile of this particular variable on changes with this particular input.

So, we can get some kind of table or plot which tells you what will be the values of say y for different x; where x is the input y is the output. So, how y changes with x in either graphical form or tabulated form whatever you might prefer. Whereas design specification tells you the exact x for which you will get a pre-designed value of y. So, that is the difference for sensitive analysis it will give a data set, it will not give a particular value. And in design specification it will find that value for which you want a certain point data for y. Now we shall understand it better with this particular example.

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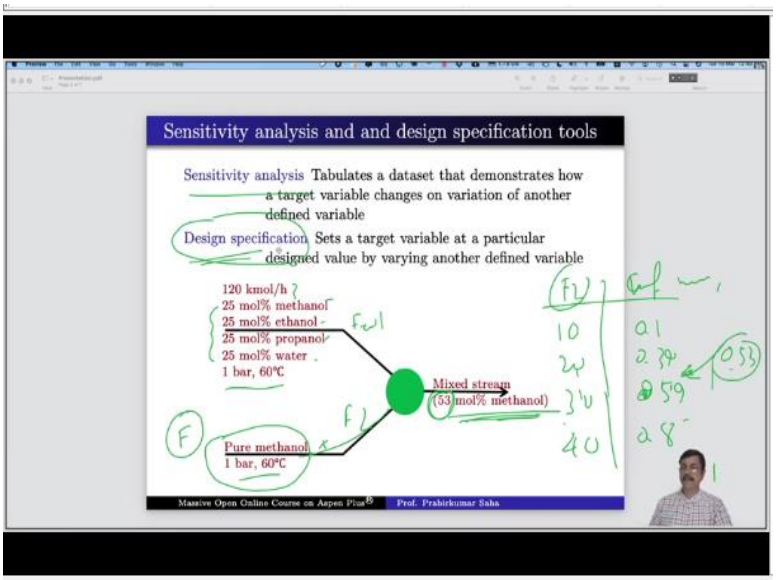

This example says that we have 2 streams, this is feed 1 and this is feed 2.The feed 1 contains equimolar mixture of methanol, ethanol, propanol and water. Its flow rate is given and pressure and temperature are given. Feed 2 contains only pure methanol with pressure and temperature, its flow rate is not given. The flow rate information is not there. In the mixed stream we want 53 mole percent of methanol.

In other words, we have to find out for which value of flow rate of this stream we will get 53 mole percent of methanol in the output. That is exactly is the design specification and what is sensitive analysis? The sensitivity analysis will say for what values of this F2, what will be the mole fraction of methanol in the mixed stream. So, for values 10 it will be saying 0.1, for 20 it will be 0.39, for 30 it will be 0.59, for 40 it may be 0.8 and so on. But it will not tell you what will be the value for 0.53; for that you need to do design specification.

So, let us solve it in aspen domain. For that go to the aspen simulation window.

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In aspen simulation window first, you have to fix the properties, here we have methanol, ethanol, propanol and water. Let us use the NRTL method. Now go to the simulation window, here first you have to bring in the mixer, connect the material stream. So, this is feed 1, we add feed 2 and this is the product.

So, we rename them let us write F 1, this is F 2 and this is P, that is product. Press next the temperature pressure 1 bar and 60 ^{0}C. So, 60 1 bar and flow rate are 120 kmol/hr. and the

mole fractions they are equimolar. They are equimolar so equimolar mixture of 0.25, 0.25, 0.25 and 0.25. Press next, feed 2 here again it is 60-degree 1 bar and it is pure methanol.

So, we have a mole fraction of 1. Now here we have to understand one thing that without giving an input to the total flow rate we cannot go forward a rating calculation of a simulation. So, we have to give an information to it. But our target is to find out for which value of this flow rate we will have the output or product quality to be 53% methanol that we will see later. But for the time being we have to give some data.

Let us give a data of say 10 kmol/hr to begin with press next. So, everything is defined, let us run the simulation, yes there is no error in the result, no warning in the result. So., we go and see the stream results of B1 and if you see the mole fractions of P it is 0.3, 0.23, 0.23 and 0.23. The methanol is 0.3, but we want it to be 0.53. Now let us do the sensitivity analysis first.

For that we have to go to this one sensitivity analysis, press new, first we have to vary something, what shall we vary? We will vary the flow rate of F2, so new type stream variable stream F2 and the variable is molar flow rate, we have to give a starting point and ending point, we have started at 10 kmol/hr. So, we begin with there and let us go up to 120 kmol/hr.

I believe within this we will get somewhere 0.53 mole fraction of methanol in the product stream and we have to give the number of points or increments let us give an increment then we will have 23 pairs of data. Then go to define, here we have to define the target variable which we want to achieve. So, we want to achieve a new thing that is called mole fraction of methanol in product.

So, we give this the name; obviously this name is a stream variable which is mole fraction in stream P of component methanol and then go to tabulate here you fill the variables, so it will form a table in which the column 1 will have the data of flow variable, the molar flow rate of F2 and in the second column we will find the corresponding mole fraction of methanol in product stream. Now it is ready to run. So, run the simulation, it is done very quickly, just go to the results.

Here you find vary F2 mixed molar flow rate, we began from 10 and we remember that we have got 30% molar flow rate of methanol and it has gone up to 120 kmol/hr and it achieved 62.5% of molar flow rate of methanol in product stream. So, this is the sensitivity analysis. Here you can even draw a graph, so this is the result graph, so just click ok, in x axis you will have the one which you have varied that is F2 and in y axis you have MFMP.

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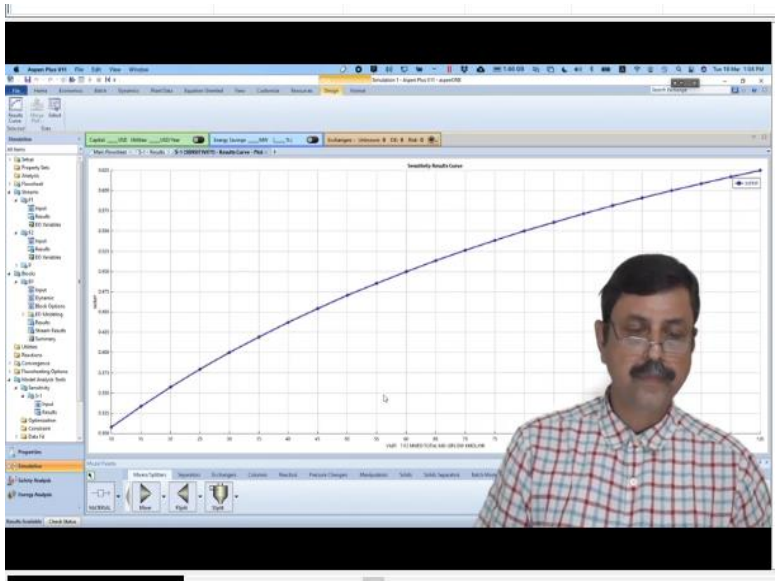

Plot it you will get this value. So, your target is 0.53, so somewhere between 0.525 and 0.55. So, 0.53 probably will be somewhere here, so it will be around 70 to 70, somewhere between 70 to 75 kmol/hr. So, if your molar flow rate of F2 is between 70 to 75 kmol/hr then you will get 53 mole percent of methanol in product stream. But exactly what is the figure?

For that you have to go for design specification. Now for design specification you have to go to the flow sheeting option, here you have design specs, just press new, design specs, again the same thing you just define a variable MFMP not necessarily you have to write MFMP you can give some other name just for the sake of understanding we are giving the same name, so that you can relate what exactly we are defining over here.

So, it is mole fraction of methanol in product stream yes, it is a stream variable which is mole fraction in stream P of component methanol, then go to next spec, so spec is you have to see the variable list. So, this is the spec, you bring it over here or you can directly write MFMP and you have to give 0.53. So, this is the target you want to achieve and you have to give a tolerance limit we give 10 to the power -6.

And then what should we vary we have to vary the flow rate of F2. So, it will be again the stream variable, stream F2 and variable the molar flow rate in kmol/hr. Now let us give lower to upper, so let us not go from 10 to 120 because we have already done the sensitivity analysis and we know that the value will lie between 70 to 75. So, let us give 70 is the lower limit and 75 is the upper limit.

So, we do not have to give you can give step size you may not if maximum step size you can fix or you can let the solver to use its own method of calculation to decide what should be the ideal step size. So, I leave it open for the solver, let us run the simulation. Yes, so go to the results, so here it has identified it should be 71.4894 kmol/hr and you will find this value in our simulation itself.

So, if you go to the simulation results you will find the block result, here you will find 71.4894, as if the simulation wants you to design this specification as per your requirement and put it back to the actual simulation. So, that is how the design goes and once that happens then mole fraction you will find 0.53 of methanol. So, this is called sensitivity analysis and design spec which go hand in hand. Sensitivity analysis will give you the range and design spec will pinpoint the value.

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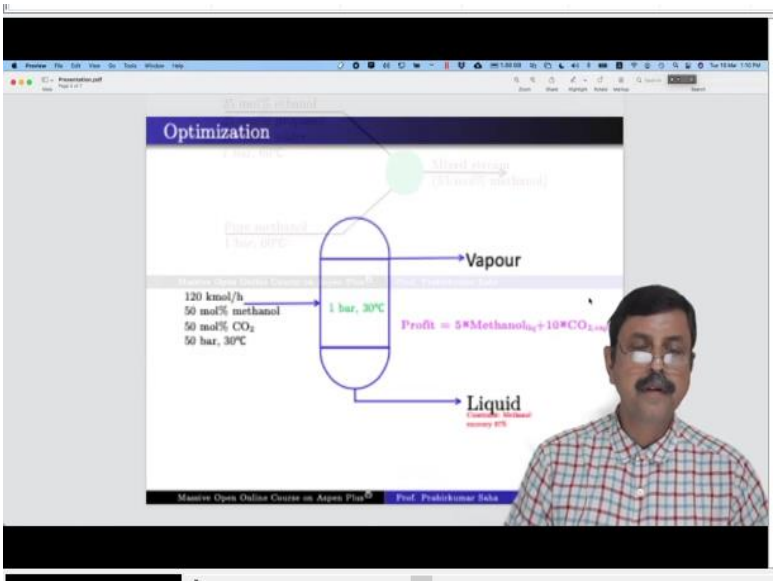

Next, we will see optimization. Here again we will learn it better with an example. So, let us take this example, we have a flash tag and we have a feed which is equimolar mixture of methanol and carbon dioxide at 50 bar pressure and 30 ^{0}C temperature, its flow rate is also given. Now it is flashed in the tank which is at 1 bar pressure and 30 ^{0}C, so you can understand that from 50 bar it will flashed at 1 bar; temperature does not change.

So, some portion will go to the vapor phase and some portion will go to the liquid phase. First let us note consider the constraint, let us say unconstrained but what is optimization? Optimization means we want to maximize something or minimize something, maximize all positive things like we may maximize the safety, we may maximize the profit, we may maximize the product margin etcetera.

And we can minimize the loss, we can minimize the effort, I mean some of the things are quantitative; some of the things are qualitative. But in aspen you have to give certain quantitative measurement, something like say profit. Now in this simulation let us take a profit figure. This profit figure is 5 times of methanol in the liquid phase plus 10 times of the carbon dioxide in vapor phase.

So, addition of these 2 is taken as the profit. So, basically, we are saying that we want to maximize this profit, so for which kind of process condition we will achieve this optimized operation? So, again let us go to the simulation window and do the problem we will learn it better.

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So, for that we have to open a new simulation, so we have methanol and carbon dioxide.

Press next, let us choose UNIFAC, run property method is done, go to simulation, here we have to bring in the separator flash tank, sorry this is the vapour and this is the liquid, so rename them this is our feed, this is our vapour and this is our liquid and give this name as flash tank, the name of the block. Now let us press next, we have to give this information.

So, it is 50 bar 30 ^{0}C and 50 mole percent of methanol and carbon dioxide each to 120 kmol/hr. So, we give 60 and 60 that will make us 120 kmol/hr per hour and the flash input we have 1 bar 30 ^{0}C. Now it is ready to run, for the time being let us not use any optimization let us run it. Now if you see the results you will find the molar flow rate of methanol in liquid is 43.5878 and carbon dioxide in vapour phase is 59.284.

So, basically, we have to have 5 times of this plus 10 times of that. So, 5 times of this and 10 times of that we have to maximize this figure. For that we have to go to the model analysis tool and say optimization. Go to optimization, press new, here you have to define. So, press new, you give it a name flow 1, what is flow 1? Flow 1 is stream variable which is molar flow rate of stream liquid and component methanol.

So, this is flow 1, we have to take 5 times of flow 1 and we have to take ten times of flow 2 which will be defined as again stream variable, molar flow of vapor CO_2 component. So, this is defined as flow 2. We have to take 5 times of flow 1 and add with 10 times of flow 2, so that will be our profit. Go to the objective and constraint at this moment let us not select any constraint we have to maximize profit.

We will define the profit later, let us write profit, go to next and vary. What we have to vary? We have to vary pressure. Now our flash tank we are operating at 1 bar pressure but we can operate it anywhere between 1 bar to 50 bar because our inlet is 50 bar, so we can tune the pressure of the flash tank. So, that our profit is maximized. So, we can say new variable is it can be a block variable which block flash tank and the variable is press, that is pressure in bar.

Now we can begin from 1 bar to say we expect that within 40 bar the result will come. You can go up to 50 bar also not a problem, but let us try with 40 bar if it is not possible we can go higher. So, it is ready to run, so run it, now here we had defined what should be the objective function. It is profit, but we have not defined what is profit. So, for that we have to write a Fortran code and as you know the Fortran code has to start from 6th or 7th column onwards.

So, first 6 columns you leave, so you begin 1, 2, 3, 4, 5, 6. So, 6 columns if you leave from 7th column you begin profit is equal to 5 times the flow 1 you can just press the right button of the mouse and you will find the variable list from there you can drag it over here. So, your Fortran code is done you have defined your profit. Now you are ready to run, so run the code. Yes, so the optimization is done, just go to the results.

So, the objective function that is the profit is 846; this is the value of the objective function. Now initial value it was 43.5878 for both the flows at 1 bar pressure and final value it is 54.5883 and final value of flow 2 is this. So, at this condition the profit will be maximized. So, just go to the manipulated variable and you will find the final value to be 2.49263 bar. Now that means at 2.49263 bar the profit will be maximized.

Now till now we have not given any constraint to the system. If you see the result of the flash tank you will find at this point at 2.49263 bar what is the mole fraction of methanol, it is 0.953046. So, 95.3 mole percent of methanol is there in the liquid phase. Now let us say we will give a constraint to the process. What is the constraint? The constraint is defined here methanol recovery in liquid phase should be 97%, at this moment it is 95.30.

So, even if it has optimized the system but we are not happy with this optimization we have to run the system with constraint on methanol recovery. So, for that we have to put a constraint over here. So, press new, here we have to give the variable name, we can give the name as con 1 that is constraint 1 and what is that constraint, constraint has to be the stream variable which is mole fraction in the stream liquid of component methanol and what will be spec.

Spec will be CON 1 that will be enough. Now what should be the specification, it should be minimum 97%, it is not exactly 97% it should be minimum 97%. So, you just say the CON 1 should be greater than or equal to 0.97. The tolerance you can give 10^{-6}. So, constraint is done. Now go back to the optimization input earlier you did not put any constraint but right now one constraint is available you have to select it and rerun the simulation.

Now do not run the simulation at this moment just reset the simulation to its original value, otherwise you will not get the correct result. So, you have reset it and then run it once again and go to the result once again. What is the value of manipulated variable? It is 1.6704 bar, the value changed to one point earlier it was 2 point something. Now it is 1.67 and at that value you see at this pressure what is the mole fraction of methanol, it is 0.97. So, you have put a constraint in the methanol recovery accordingly you have redone the optimization and found a renewed result which is constrained optimization.

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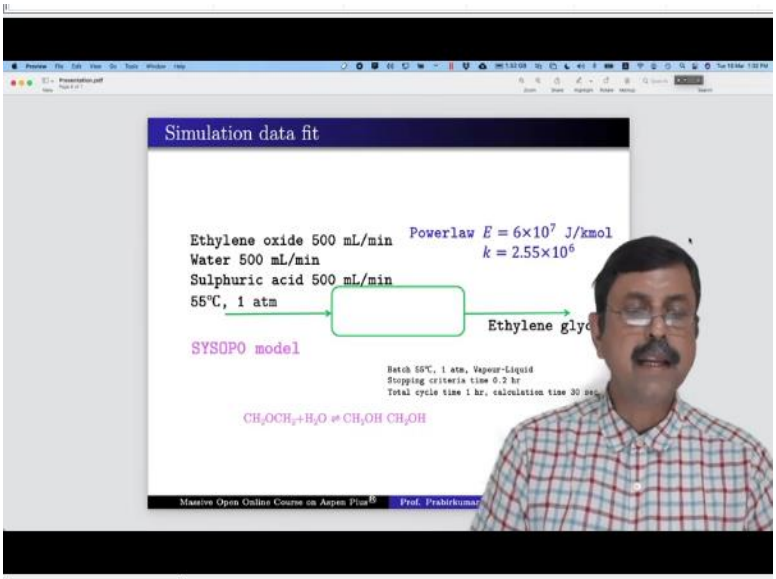

Finally, we will do the simulation data fit. Suppose if these are the experimentally found values then what will be the process parameters which will guide the model simulation through this experimentally found values or as close as them. So, this is simulation data fit. Now we shall learn the simulation data fit with this simple example. It is an example of a batch reactor which operates at 1 atmosphere pressure and 55 ^{0}C temperature.

Now the input to the batch reactor is ethylene oxide, water and sulfuric acid as a catalyst, temperature is 55 ^{0}C and 1 atmospheric pressure. Now as batch reactor we do not have any significance that per minute condition but as you know that aspen plus needs to have a flow rate information for the system input. So, we have to keep this per minute thing over here. We will use this SYSOP0 model and the reaction that happens inside is this is the ethylene oxide plus water it forms ethylene glycol.

This is ethylene glycol and here sulphuric acid acts as a catalyst. Now we will follow the power law in which the activation energy is 6*10^7 J/kmol and this parameter is 2.55*10^6 and the stopping criteria for the batch reactor is 0.2 hours. Total cycle time we can say 1 hour and calculation time each 30 seconds, after every 30 second we will pick up the data.
So, let us first run this simulation and check what happens.

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For that let us go back to aspen simulation and open a new stimulation block. So, we have to find ethylene oxide, this is the one and then we have ethylene glycol, this is the one. So, we rename it. We write it as ethyl oxide and we rename it as ethylene glycol and then we have water and sulfuric acid.

Press next and we will use this SYSOP0 model, press run, go to simulation. Now go to the reactor, pick up the batch reactor, connect the streams, so rename the streams, so just rename the stream as feed product and r batch, then press next, well so it is asking for inputs for feed material which is 55 ^{0}C 1 atmosphere pressure and we have the flow rate of 500 ml/min for all of them.

So, we have flow rate ethylene oxide 0.5, water 0.5 and H_2SO_4 0.5, it is done. Go to next, so operating specification it is a constant temperature operation at 55^{0}C, specify reactor pressure let us say it is running at 1 bar. For the time being do not use sulphuric acid we will see later. Go to kinetics, we have not defined any reaction so define a new reaction r 1 which will be a power law type.

So, go here define it, say new. So, the component is ethylene oxide reacts with water and the product is ethylene glycol, its coefficient -1 and -1 because they are reactants and this is the product with exponent 1. And go to kinetics here the k value it is 2.55*10^6 and E value 6*10^7 J/kmol. So, it is done. Go to next, stopping criteria.

So, the only criteria that we can think of at reactor variable time and let us stop it at 0.2 hours. Go to next, operation time total is 1-hour, maximum calculation time again 0.2 hours an interval in seconds 30 seconds, no it is wrong, so run it. So, we can see the result. Go to profile of the batch reactor and you can find the composition over here. So, let us write minutes, so 0.5 minutes, 1 minute, 1.5 minutes because every 30 seconds we have recorded the data.

So, how the ethylene glycol is produced and coming to point of steady state that is the final product. So, for 12 minutes we have taken, so let us plot the data composition, so reactor molar composition of ethylene glycol.

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So, this is the plot that we have got and if you set time in minute then we can understand how the molar composition or mole fraction of ethylene glycol changes with time and within 12 minutes it reaches almost the final value. Now this is the model performance, but suppose we have got a set of experimental data and this model performance we have got by giving some values suppose the activation energy or the reaction constant k value. Those are the figures that we have given, but if we have some experimental data points of time versus glycol mole fraction of this nature.

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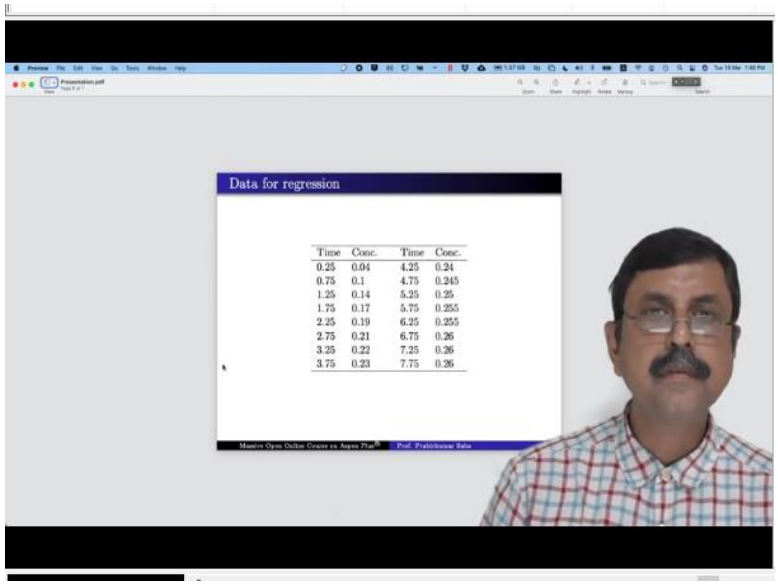

So, we have time versus concentration of glycol, time in minutes and concentration in mole fraction rather. So, we have got time versus concentration, that is the mole fraction. So, time

in minutes and this is the mole fraction. So, this is the experimental data for regression. For that we can enter the values in the data set. So, for that we have to go to the model analysis tool once again and here we have the data fit.

Press new, type of data profile data because we do not have a single point we have a complete profile, so write profile data, r batch, the block name is also r batch we have given the name r batch and what is the variable name we have to give some name to the variable. So, let us write mole fraction of ethylene glycol and the variable name is mole fraction in liquid phase component ethylene glycol set.

Go to the data, here you have to add the data instead of hours we write it minute. So, this is the time and this is the mole fraction of ethylene glycol. Now here let us put the time first, for that we write it here in this fashion. So, it is 0.25. 0.75, 1.25, 1.75, 2.25, 2.75, 3.25, 3.75, 4.25, 4.75, 5.25, 5.75, 6.25, 6.75, 7.25 and finally 7.75. Then we write the concentration values first is 0.04 then 0.1, 0.14, 0.17, 0.19, 0.21, 0.22, 0.23, 0.24, 0.245, 0.25, 0.255, 0.255 again, the last three are 0.26, 0.26, 0.26.

So, this is the data set or say experimental data set that we have got. Now if we add it to the curve of the previous plot, now this is the MFEG result. So, this is the experimental result that we have got. Now we have to build a model with all its parameters which will follow this particular experimental data curve as close as possible. So, that is what regression is.

For that what we need to do; we need to go to the regression. In the regression we have to press new data regression and press the data set ds 1, vary new variable, what should we vary? Let us vary this particular one the k value, k = 2.55 10 to the power 6. Now this is the model parameter. Now we have the liberty to change this to match with our experimental data set.

For that let us vary this one which is a block variable which block it is r batch, no we do not have to use block variable we have to say reaction variable. So, it is not actually block variable it is reaction variable, so it is reaction variable and which reaction it is only one reaction is there r1 and it is the not activation energy it should be the pre-exponential factor in SI unit give then ID as 1.

And we have to give an upper limit and lower limit, so the value actually is $2.55*10^6$. So, we can give from 2.4 to 2.6, so $2.4*10^6$ to $2.6*10^6$. So, we assume that or we envisage that the result will be available within this. We go to convergence, here the absolute function tolerance it is too high, let us change it to $1*10^6$ and go to advanced.

Here the initial step size is 1, let us make it higher 1000 and then run. So, it has run the simulation, find the result. So, you can see the manipulated variable is $2.4897 *10^6$. So, its initial value was 2.55 it has found it to 2.4897. So, if you go to r batch, go to kinetics, go to input. So, if you go to r 1 kinetic instead of 2.55 if you write $2.4897*10^6$.

Press reset and for the time being let us deactivate. So, it will not do any problem and press run. So, we have put the value that we have obtained from this result and let us see what result we have got. So, this is the profile data in minutes. So, this is how the ethylene glycol changes with time let us plot it composition ethylene glycol. So, let us change it to minutes and now you go to the data set. And then add this curve with the already plotted curve and you add them in a single curve, a single axis.

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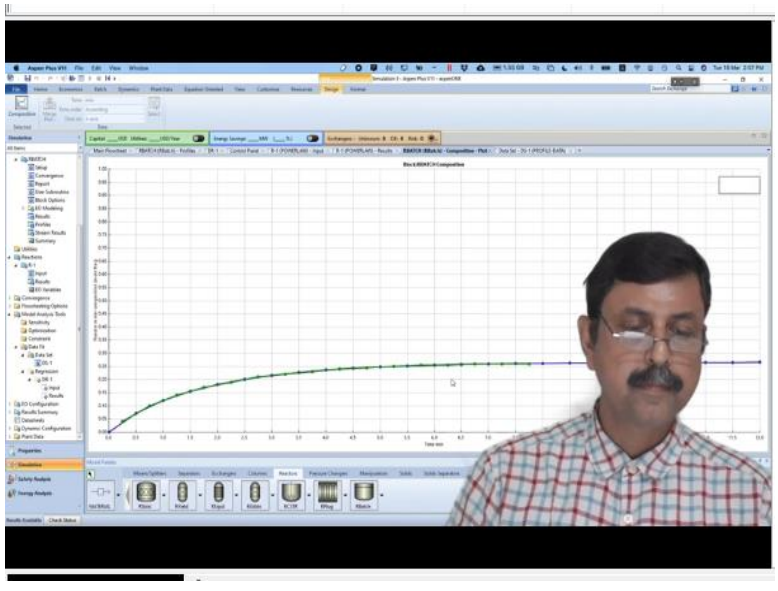

Now you can see how they are matching. So, this is the green line, it is the experimental result and blue line is the aspen mathematical model simulation result, taking the values of k value which, it has optimized or which it has regressed using the experimental data. So, that is how we do the simulation data fit. So, we end our lecture at this point today thank you.