Principles and Practices of Process Equipment and Plant Design
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Module - 05
Lecture - 62
Process Design using Simulators

Hello, good day to you all. So, today we are going to speak again, towards the end of our course, we are going to detail today and have some idea about Process Design using Simulators, the process simulators. We have talked about the basics of process design and design process in general; we also have talked about what exactly are the communication details and what are the basis documents generated.

And we will start from that particular point, that is we start with design; we see how to evaluate a design, we know what simulators are, then we see how simulators can be exploited for the stage of, at the stage of design and we also see one very interesting modern aspect, that is so far what all approach to design you have taken is based on equilibrium stages. But, we will also have here on a rate based approach; we just know what it is, because modern simulators come with a facility for rate based modules as well. So, we start.

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The moment you talk about process design, possibly you are talking about a plant, which will be built with several equipment and they will be connected. If you look at the design calculations, many of the design calculations are straight forward; for example, if an expression is given and the parameters which constitute the expression its values are known as design inputs, you simply calculate and evaluate the expression and find out the output. So, that is a top down approach.

In some cases, the expression of the output that is to be generated as design output are not available in explicit forms of formulae or maybe functions. So, they are implicit functions. So, they have to be solved in most of the case in a, iterative fashion. So, the design calculations and you have definitely come across both type of such evaluations during your design stages of different, well stage wise separation processes as well as a heat exchanger design.

In fact, your heat exchanger design is a good example of the iterative trials involved. You assume a thing, you evaluate certain other parameters, check back whether your assumptions are correct or not; if not, you iterate once more. We also have seen that your design output should be optimal.

And here whenever we have said optimal, we have meant truly that it should be an economic optimum; of course we know that it need not be an economic optimum by evaluating an economic parameter like profit or cost, it could be another parameter like an efficiency which could be maximized with the same aim.

There is one more thing which is there, that is my finalized design should be stable. In most of the cases you land up with several design alternatives; may be two, three or four, rarely, you have a unique solution. So, quite naturally when I say or when I find that optimality wise you have more than one solution which is giving you the same efficiency or benefit in terms of financial parameter, you have to come, you have to compare these between these and design and choose the most stable one.

So, there is a question now how to evaluate quantitatively if a design is stable. Well before you decide if a design is stable or not, you ask certain questions, those are mostly heuristic ones. For example, it could be which option is easier to maintain, which option will take a lesser time to build.

And after that even if we have some option left with us, we normally have to compare between these options quantitatively, which one is more stable. This concept we have just mentioned in one of the earlier classes, but we will try to understand it in a better way.

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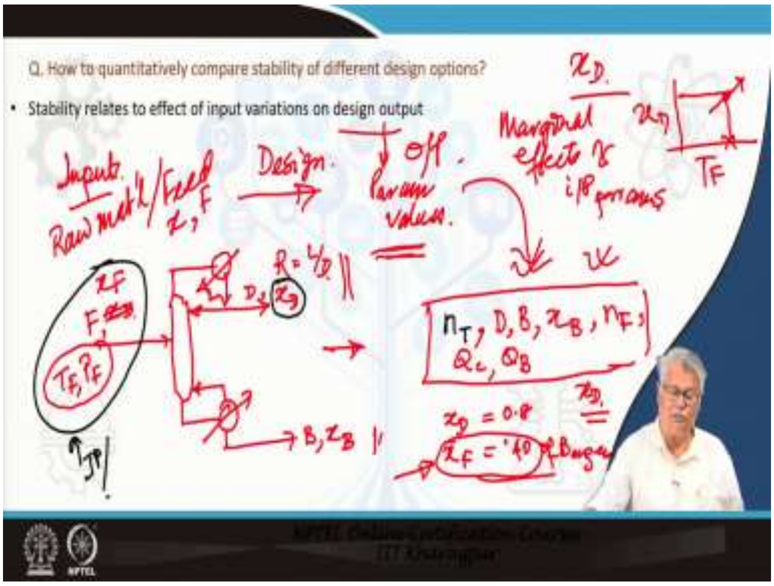

Let us see that. The question now is to how to quantity quantitatively compare the stability of design different design options. See whenever you are designing something, there is a design output; that means a set of parameters, parameter values which are from the design outcome, this is based on your inputs. What are the inputs? It could be something related to the raw material or the feed; it could be its compositions, its flow rate.

Similarly, it could be other several other parameters also. Now, based on this you have generated using the design process, the final design output parameters. So, suppose such a parameter in case of a distillation column design if we see; what all it will it be? I just have a distillation column here, I have a feed rate F, I have a condenser; I have here a reflux ratio, which is nothing but L upon D.

My reflux ratio is L upon D and my D has got a composition x D and here I have a reboiler, where I add heat, generate vapour. I mention the, maintain the temperature here and I take out a bottom product B with a composition of x B. Naturally my feed composition is x D, which is available at T F the temperature of the feed, pressure of the feed is P F and these are the ones, ok. So, actually it should be x F. So, it I just corrected here as x F.

Now, what are the outcome of design? I let us see there are two types of parameters here, you will what you will find here is something like this; I have based my inputs on these, I also have based on a desired distillate composition. So, my black circles are covering the parameters which are input. So, these are my input parameters.

What is my design output? By number of trays, I will use another colour to distinguish let us see; this is the number of trays, you have found out the distillate flow rate, the bottoms flow rate, the x t is definitely known to you. So, I have found out my x B also. And also I have found out for maintaining this corresponding to this particular number of trays, what is my feed tray location; also what I have here is my Q C and Q B, which are the heat loads here.

So, from my, this designed process, I generate these as output parameter values. Now, there is one thing; suppose it is a simple case of benzene toluene which we always use in the undergraduate class as an example, we normally say my feed composition is roughly 40 percent benzene. So, it is 0.4 mole fraction of benzene and I want to distillate composition of 80 percent benzene, which is 0.8.

Now, when I say and I do a design problem, I have assumed an unique value of x F. Similarly I have assumed some specific temperature here of feed, which I am assumed that is coming from a tank temperature of T F; the pressure we have assumed to be roughly about 1.5 k g per c m square gauge or so from a pump and based on that, we have found out one set of output here.

Now, let us look at the output here, apart from this; I mean in order to what is this corresponding to, this is required to obtain a composition of x D, which is my functional requirement. Now, once I have designed this, let us see; though I have designed with my best estimates for my input variables, if I actual practice, if these parameters change slightly, what will be their effect on the final design parameters or final performance of my equipment?

Now, the final performance of my equipment is based on x D. So, quite often what you normally do is, you will plot a parameter which could be maybe the effect of T F on x D and this being the design, this x D is basically the design value. And if it changes, you may have a parameter variation like this.

That means if my T F increases by 3 degrees or 4 degrees around my operating around my design point here, my x D will correspondingly increase or decrease this will happen, keeping all other parameters. This is the way we find the marginal effects of the input parameters; but unfortunately we are not always so fortunate, I mean this is not always the case. Now, what we see here is, we I think I need to add one more slide here, I will do here and then carry on, you will do that.

Student: First we are going to (Refer Time: 12:02).

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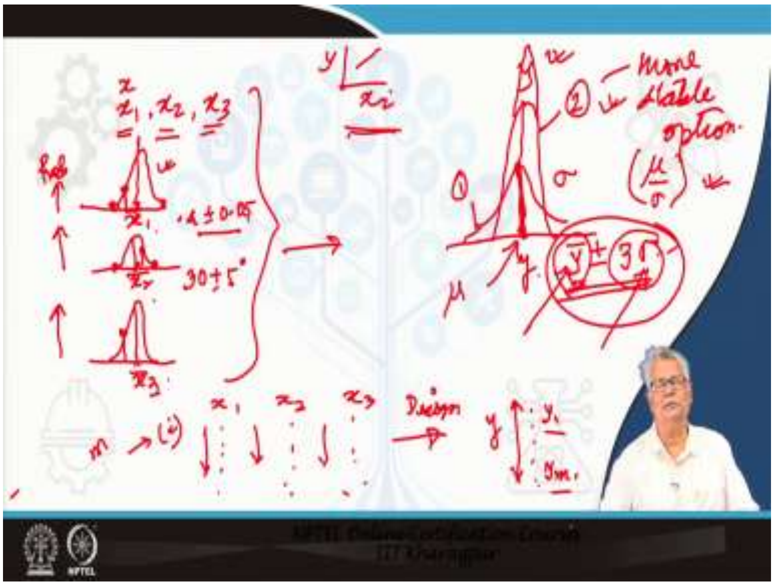

So, here what we have is, I put it like this; if my input values are x and my output parameter is y, I will have several parameters x 1, x 2, maybe 3 input parameters and say for the moment we are observing only one output parameter y. And what we have seen that there will be if I have only the variation of x 1, x 2 or x 3; we can run three design cases and naturally we can plot a x versus y plot.

Quite expectedly this will be something like this for possibly for x 1; for x 2 it will be something else, for x 3 also it will be something x something else. Now, in reality whenever you are talking about x 1, x 2, x 3; what we have done is, if we look at the scale of their operation, I have chosen the most probable value of x 1, the most probable value of x 2 and the most probable value of x 3. This basically is naturally the probability.

And I have generated my design here, my design output in this particular case is y; based on the best values of x 1, x 2 and x 3, which could be either the best estimates or the average, around which there will be variations. If it is possible, it in fact it happens most of the time; even if I say my feed will contain 0.4, it will actually be 0.4 plus minus 0.1, 0.05 say.

So, this particular point and this particular point will not be 0.4. Similarly, if I talk about a temperature; the feed temperature could be say 30 plus minus 5 degrees, so this will be 35, this is 30, this is 25. Now, in case of marginal variation what we did is, we have kept all others constant; but in reality all these parameters will be having their natural values, which are randomly varied, but each individual parameter will have its own probability distribution.

So, what you can have or what you will actually find is, there will be different combinations of x 1, x 2 and x 3; one could be here, the second value x 2 could be here, the third value x 3 could be here, that means this is a combination of x 1, x 2 and x 3. And if I randomly generate the values of these, such that the standard deviation and the mean values are x 1 bar, x 2 bar, and x 3 bar as it is shown here, I have a set of input data here.

In all these cases if I use my design procedure, I will be generating what? I will be generating several values of y. So, and this y value will also have a variation. So, what I do now is, I do exactly the same thing; I have a set of values of, suppose I have done it for n number of times or rather m number of times.

So, I have the values starting from y 1 to y m. I simply have a distribution curve here, which looks like this; that means it is just a frequency curve in this particular case. And in this case what I find here is, y bar the one with this maximum frequency or probability is my most probable value of y and its variation will be given by the standard deviation here.

So, your actual output will vary between y sigma, sorry y bar plus minus 3 sigma; provided that distribution assuming that distribution is normal, which is in most of the cases. And here there is one thing very specific; if you are considering a normal distribution, 99 percent plus it is 99.7 percent possibly will be your varies of y, which will lie between y plus minus 3 sigma.

So, if you have this plot and if you specify this y and specify the sigma value of your output for different outputs; you definitely can say that most probably you are going to operate with a value of y bar with this particular design, but there may be some variation with respect to y, which could be plus minus 3 sigma in this case. I just generalize it a bit, I call this value mu which is standing for the average.

And suppose I have two cases of design which I am comparing; one gives me a sharper value, this the first one is number 1 design, this one is number 2 design. Now, it is obvious that my second design is less affected by the random variation of the input parameters; that means even if my input parameters deviate from the design case values within normal limits, my output parameter will remain fairly, ok.

And how is this parameter decided or; that means my second option is a more stable option. And how do we decide it? Because if I look at mu upon sigma, this is going to tell you how thin this is going to be; if this is small, your sigma is small. So, naturally you are expected to have a very narrow and a tall curve like this.

So, lower the value of mu by sigma, your design is more stable and here by more stable and this is a quantitative measure of having an idea that how stable is your design output and with this you can compare different options of design and opt for the more stable design.

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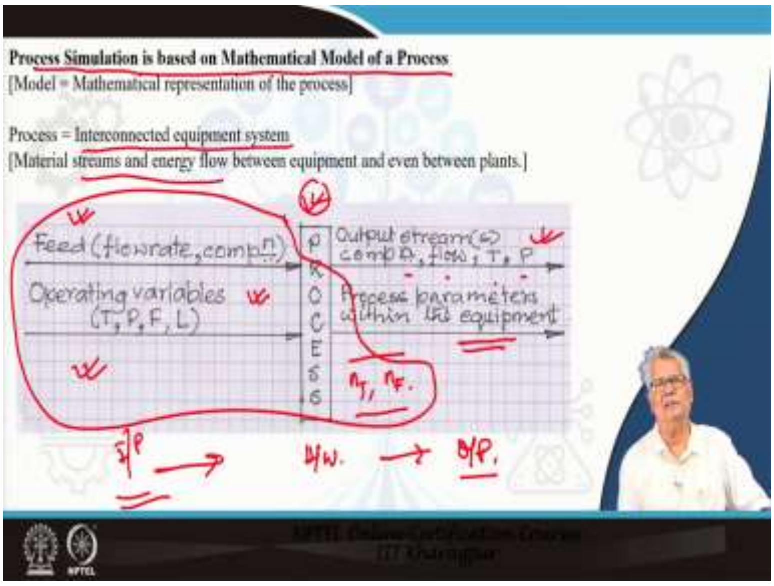

Now, we are coming back to the old question that is process simulation. This is perhaps a new term in this particular class and here I just have to say a few things before we start truly. Process simulation is based on mathematical model of a process. In a process what happens; you have the process itself, may be the distillation column with its all associated equipment.

You fix the feed rate, you fix the operating variables of; that means the column top temperature, reflux ratio everything is known, your process means your number of trays affects, your feed tray is fixed and naturally your heat transfer limits everything is fixed, that means you have your specifications of your hardware.

And in a plant what happens; if you are given the plant, whose hardware is given to you. If you know your feed rate and if you operate your plant with the known operating variables; you definitely what you do is, you obtain the output streams, whose composition flow rate temperature pressure you come to know.

Not only that, you know quite a few other things also. In your distillation design for example, using McCabe Thiele or rather everything related to similar operations. What you certainly know is, you know the tray to tray flow rates, you know the intermediate tray temperatures and things like that.

So, what I would like to say here at this particular point, your process is basically the hardware, it is basically the hardware and you have a set of inputs which generates a set of output from your process and you can verify your process goals or process functionality.

Now, in a process you will have different equipment, you have the overhead condenser, you have the reboiler, you have the column, you have a pump everything. And all these equipment are interconnected in your plant in a as a system. And between these the streams and energy flow between these connections and connected equipment and sometimes even between plants.

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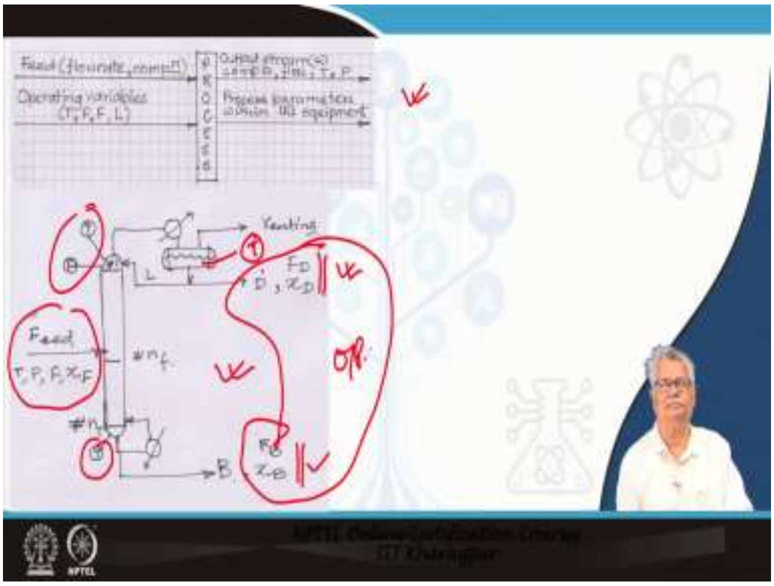

Now, suppose we take this case a little bit further. In this case what we have, I have just drawn the same example which I have shown here earlier and I have tried to give you an idea about the plant and this. So, what are the feed?

The feed details are given here; the operating variables are all these temperatures that you can see and naturally you have a temperature here also, which is also known here, because you can manipulate and find out what exactly will be the pressure here as well. And what you get are these things; it is nothing but you can compare with the earlier slide and you know that these are your output variables.

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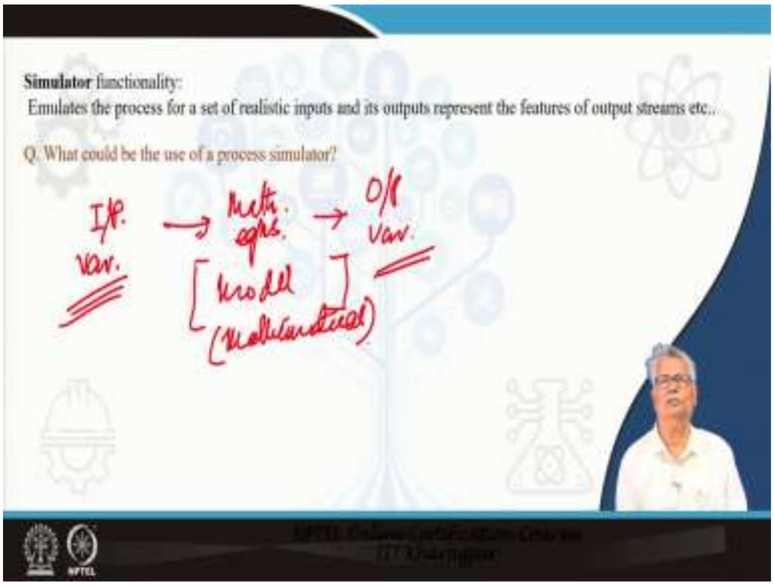

Now, we move one stage further. Suppose instead of a process you have a set of mathematical relationship, which connects the variables, which states the relationship between the variables. Then what happens is, if I know my input variable values and if I know my mathematical equations that connect the variables; then I can always find out the output variables and this set of mathematical equations is my model, often known as mathematical model.

Now, what I would like to say is, so a simulator is one in which if you give the realistic input variables and we know by now that what these realistic input variables are; you can find out without running the plant, the operate output features. Now, what we tried in our design is to find out the output based on my inputs; something similar is also possible here, but without running the plant, without going into the details of the exact design equations.

But it is obvious that the model equations will be almost same or the same equations in a different form in order to find out the output variables here. Now, these output variables need not be only the design output; it may be other parameters also, we will see what these are.

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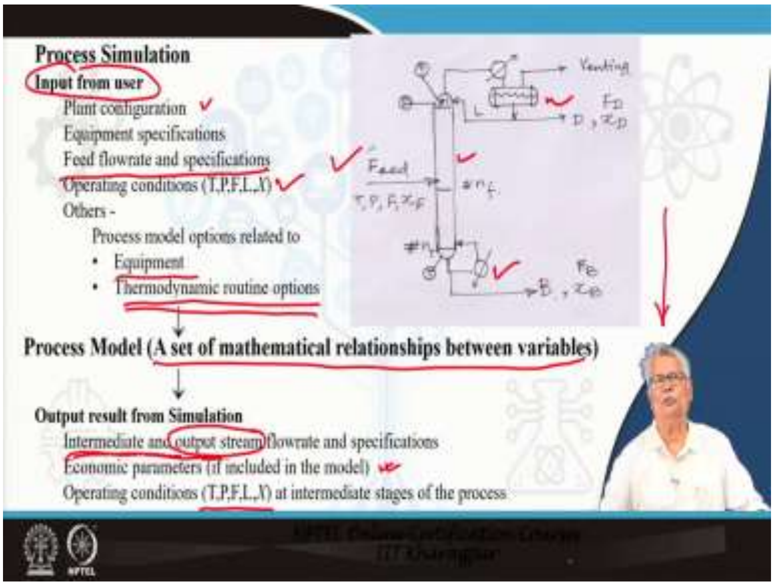

So, let us look at the steps of process simulation. Naturally you have to simulate a plant, so you require the plant configuration; here you have the distillation column, this the overhead condenser, the reboiler such thing. And the specifications must be known. You need to know the feed flow rate and the specifications of the streams which are entering as input, which is this.

You need to fix the operating conditions, the temperature pressure flow and composition wherever required and here in this case my reflux ratio which is L by D is one such parameter. You may also have to fix for your calculations how to perform the calculations.

For example, you definitely are aware that you have used different types of equations during your distillation design. You have used the shortcut method, you have used methods for your multi component, you have used the McCabe Thiele method and there could be many few other methods also.

And there you have very intimately used the thermodynamic properties and this choosing these thermodynamic properties belong to the process model options, where the equipment modelling you may have to choose whether to have a shortcut model or a detailed model of a particular equipment. And regarding the components, you are also to specify the thermodynamic routines to predict their properties and predict their behaviour like vapour pressure and relative volatility and things like that.

Now, once this input set is over, the process model which is nothing but a set of mathematical relationship between the variable takes over, it solves it. And what do we get from the output of simulation? We get the output streams, we get definitely the output streams and also a few intermediate stream details. For example, tray to tray flow rate of the vapour and the liquid.

We also may get something like the economic parameters if included in the model. We also may be requiring some other temperature and pressures at different points of your plant. So, this is basically the process simulation and the process goes top down from here and you already have an idea that what its output are going to be.

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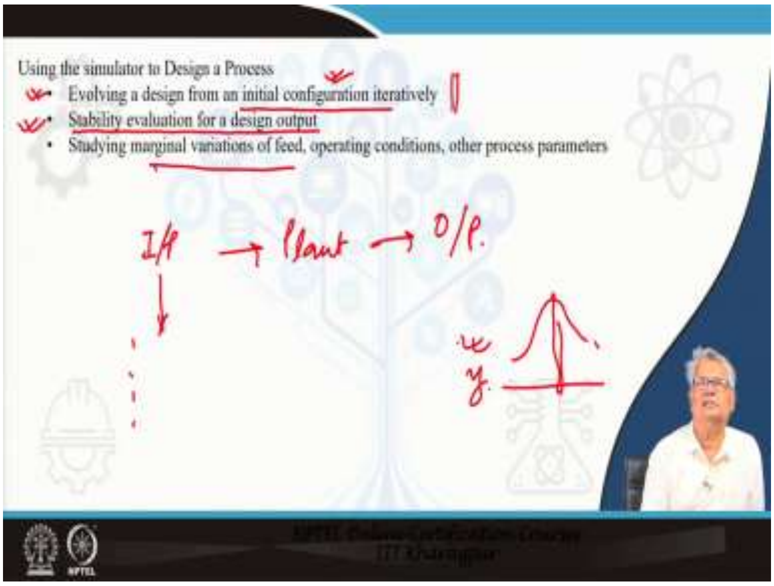

Now, the question comes how to use the simulator for designing a process. We in most of the case whenever we are confronted with the design problem; we make first a conceptual design, which leads to an initial configuration. Then what we do; we keep on refining it iteratively.

We start improving it by making changes and evaluating the effect of the change. Can I do this in a simulator? Yes, we can; because if I change my input, so if I change my operating conditions, what happens to the plant output actually is given out by the simulator. So, your processes go for an initial configuration first, simulate the process, change the parameters of simulation, evaluate the result of change and improve the design iteratively.

So, normally what you will find, your simulators are used in a design process this way; you can also evaluate the stability of a design output, because the simulator can definitely tell you what is the effect of a set of input, a set of input on your plant in producing the set of output.

So, you can run the simulation for many number of times, the m number of times that I have measured, with the variation of the input variables within plus minus 3 plus minus 3 sigma. Evaluate and find out the distribution of the y, evaluate and find out the distribution of y and possibly we with this we can say that, well this particular design is more stable as compared to the other. So, definitely we can also do stability studies.

And obviously, I did not state that the marginal variation effects of the feed, operating conditions and other process parameters including the financial calculations can be done using the simulator also.

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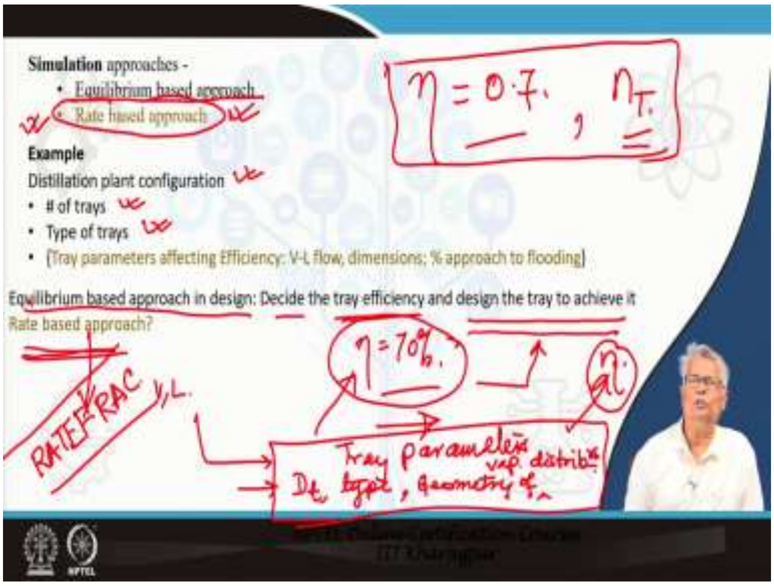

So, basically the simulation so far that I have talked about and in the design as well. So, far we have based on the equilibrium based approach, it is a equilibrium based approach. What we did? We assumed that every stage will be in equilibrium; thermal as well as the mass transfer equilibrium. Then what we do? We account from the inefficiency by introducing the term efficiency and then we go and arrive at a design.

There is another approach which is called rate based approach, we will discuss this immediately after this. An example of this is again the same thing, which we have discussed, the distillation plant configuration we have; it tells us what, it tells us the number of trays and the type of trays.

Now, in case of equilibrium based approach in design what we do is, we decide a priory a value of tray efficiency, maybe we will assume eta is equal to 70 percent. We take a particular type of tray, assuming the value of efficiency to be 70 percent; we find out the ideal number of stages, we find out the actual number of stages based on 70 percent. And then what we do is, we design the tray to achieve 70 percent. So, this is the typical approach that is taken in case of equilibrium stage.

In case of the rate based approach, the rate based approach it is different. In fact, in the rate based approach, it is possible for you, rather only if you can evaluate this while you are designing itself; that means here during the design itself, you generate the tray parameters.

What are the tray parameters? Possibly the diameter of the tower, the type of tray, the geometry of the vapour distributors on the tray. And if you know this and since you already know that, you can find out the intermediate tray vapour and the liquid traffic; if you have during your process itself the vapour and the liquid traffic given to you, from here it can definitely generate the efficiency value.

So, what you do in a rate based approach is, you account for the actual efficiency here and then proceed with your design. Now, this has not been the approach and it is a more recent approach to design, which was not there in the earlier simulators. And an example of this is definitely the modules, where you have such equations built in, which can do this type of calculations; that means it can evaluate the efficiency of contacting or similar parameters, while the calculation proceeds.

Now, there is one thing here, what is the advantage? In case of equilibrium base stage design; what you had done, you had fixed out an efficiency of 0.7. In the previous example what I have said. And you had proceeded and found out the number of trays. But in this case, you are finding out the efficiency of every tray, the actual estimated efficiency. So, you can go more close to the real operation.

In most of the cases, in equilibrium based, where you have assumed an efficiency value of 0.7 for all the trays; you will be keeping a good margin, here this margin could be even less, you can go close, you can calculate close to the real operation. So, that is the advantage of the real rate based approach.

And the rate based approach is in aspen plus module is for such separation using distillation is rate frac. So, if you are using the rate frac module in that particular aspen plus which has got rate frac, which you have to buy separately in fact. In that case, you can go to a more close design and a much better simulation quality. I think I will stop here with this.

Thank you.