Plant Design and Economics
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Lecture No -34
Reactor Synthesis for Complex Reactions by Attainable Region: Example - 2

Welcome to lecture 34 of plant design and economics. In this module, we are talking about reactor network synthesis. In our previous lecture we have seen the application of Attainable Region for manufacturing of malic anhydrate. That was a relatively simple example as a single p effort trajectory was enough. Today we will see a little more involved example.

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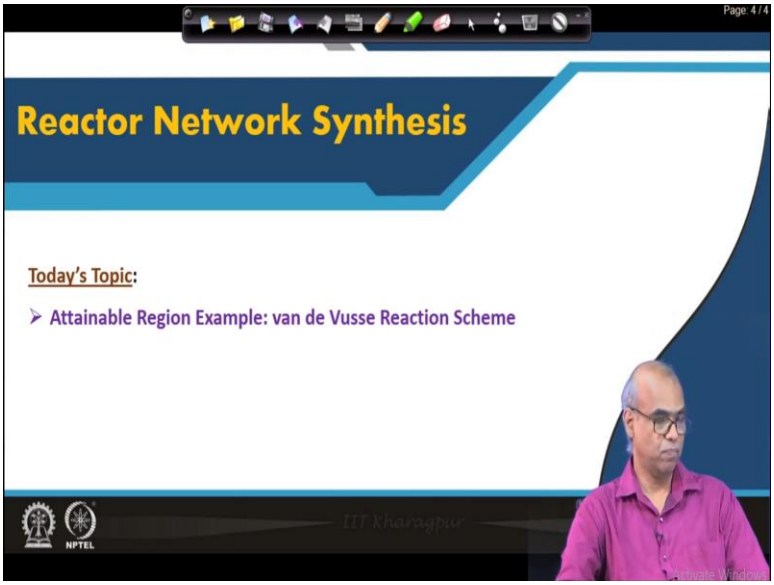

Specifically will today see Attainable Region Example on van de Vusse Reaction Scheme.

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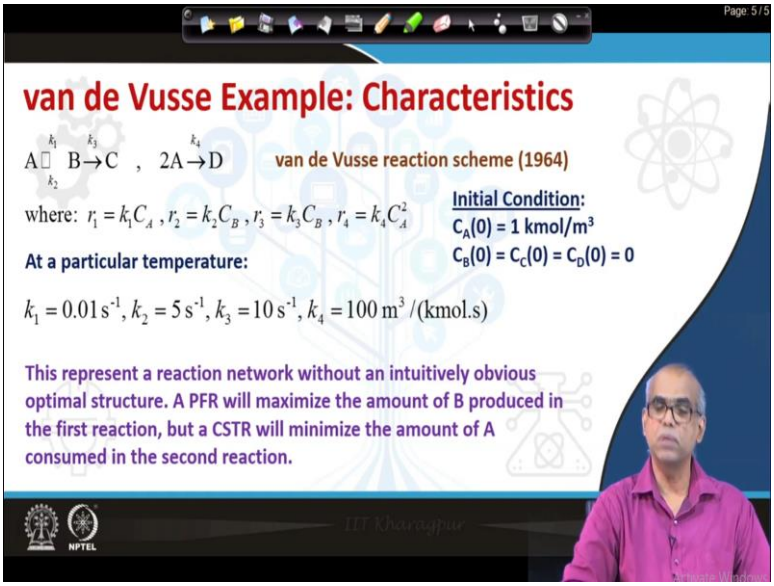

So we will use the shown liquid phase, constant density, isothermal reaction network to illustrate that Attainable Region approach. The reaction scheme known as van de Vusse reaction scheme is basically parallel decomposition of species A. So this represents a reversible reaction. The rate expressions are given. The values of the k1, k2, k3 all the rate coefficients are given at a particular temperature.

The initial condition's are given, we start with pure feed A 1 kilo mole per meter cube, and concentration of B C D all are zero at time t equal to 0. The objective is to determine the reactor configuration that maximizes the production of B for a given amount of pure feed A. Now, there is a reason why van de Vusse example has been chosen. This is a well started system, this represents a reaction network without any intuitively obvious optimal structure.

It is not easy to intuitively find out what should be the optimal reactor structure for this reaction scheme. A PFR will maximize the amount of B produced in the first reaction whereas, CSTR will minimize the amount of A consumed in the second reaction. So we will try to find out what should be the optimum reactive configuration using Attainable Region method.

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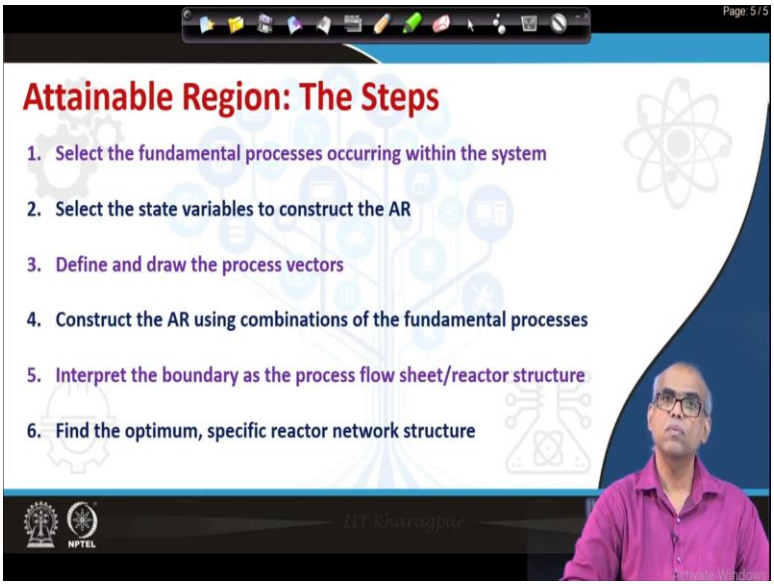

Now, these are the basic states that will follow to construct that enable region. First is we select the fundamental processes occurring within the system. We already said that the fundamental processes that will consider here a reaction and mixing. Select the state variables to construct that Attainable Region. Define and draw the process vectors. Construct that Attainable region using combinations of the fundamental processes.

Interpret the boundary as the process flows sheet, reactor structure. Find the optimum, select reactor network structure. So these are the states we will follow. So now go step by step and try to construct that Attainable Region for the van de Vusse reaction scheme and then we will find out the optimum. Our objective is to maximize the production of B.

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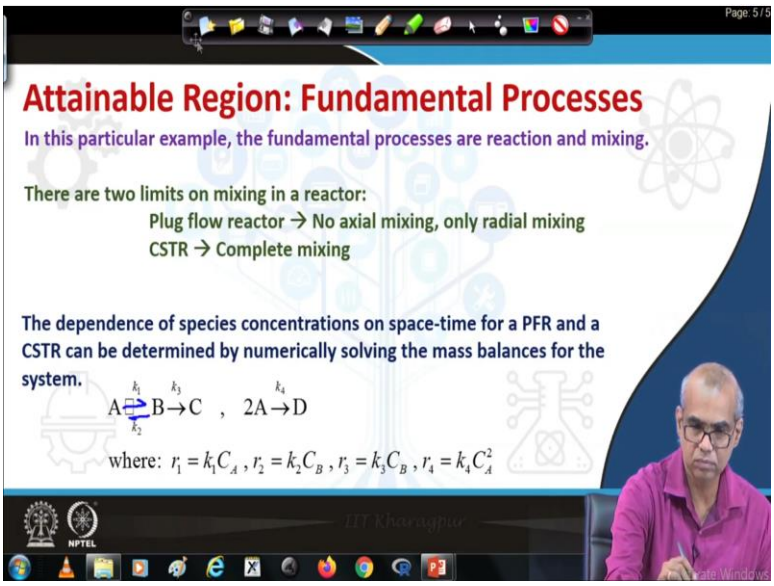

So what are the fundamental processes for the system that you are considering? Reaction and mixing. Note that there are two limits on mixing in a reactor. Plug flow reactor, which has no axial mixing and only radial mixing. The other extreme is CSTR which represents complete mixing. The dependence of species concentration on space-time for a PFR and a CSTR can be determined by numerically solving the mass balances for the system, that means for the van de Vusse reaction scheme. Again, note that this is reversible.

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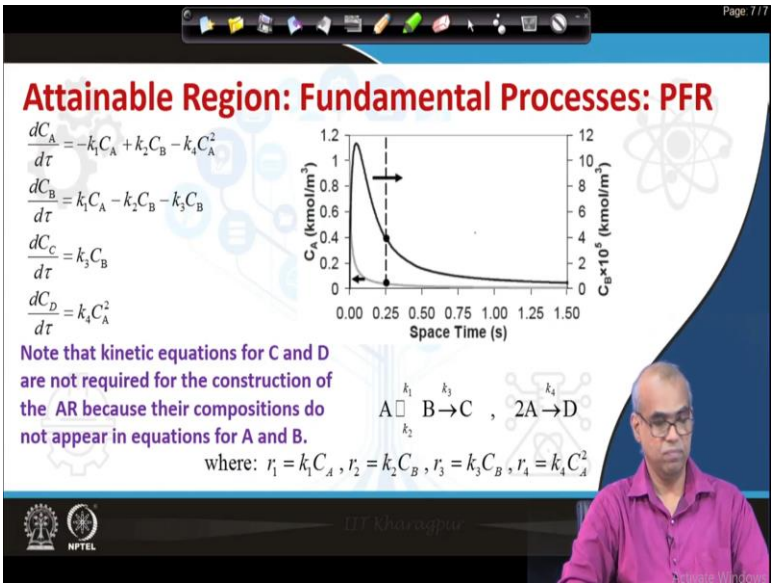

So, these are the mass balances equation Poppy effort. So, these are differential equations of the species A, B, C and D with respect to space time tau. Now we have to maximize the amount of B. Now look at the expressions or the differential equations for A and B. The kinetic equations

for C and D are not required for the construction of that Attainable Region, because there compositions do not appear in equations for A and B.

So in the first two differential equations if you concentrate you see there is no presence of concentration of C and concentration of D. So consideration of C and D is not required for developing the Attainable Region for this process. So we solve numerically, the first two differential equations with the given values of the rate constant scales, and the initial condition on k.

So this profile represents the concentration of A with time, with space time whereas this represents the concentration of B with respect to space time tau. Now you already know that this graph can be used or the data obtained from this solution can be used to present the concentration of A and B on concentrations space diagram CA, CB diagram.

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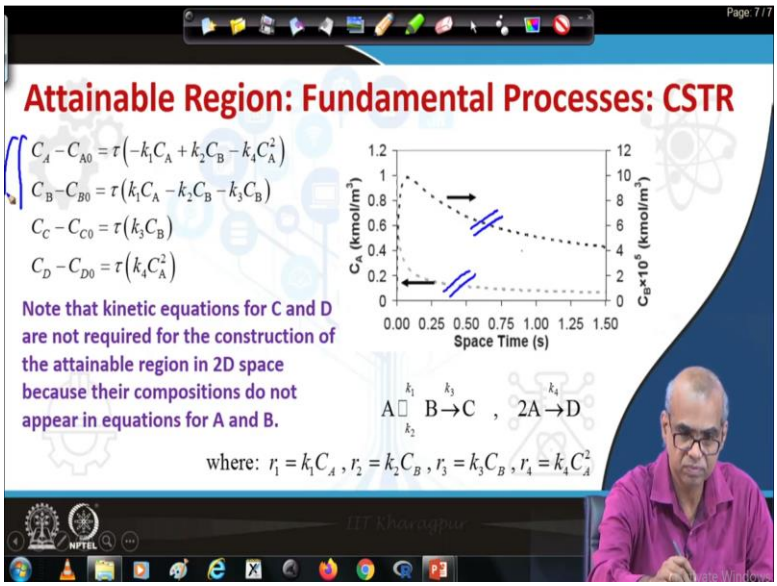

Now let us move on to the next fundamental process CSTR. Again we need to worry only about equations for A and B. Because the kinetic equations for C and D are not required for the construction of the attainable region into this space, because they are compositions do not appear in the equations for A and B. So focus your attention only on first two equations. Note that these are algebraic equations.

Whereas we solved differential equations in case of plug flow reactor and even we solved the differential equations we get continuous solutions of concentrations with respect to space time. Here for given values of tau, we can solve this first two equations and can find out concentrations of A and B. So these are those solutions. So for different values or space time we have solved these first two equations and then can generate this plot concentration of A versus space time and concentration of B versus space time.

Note that this figure will also be used to find out the concentrations of A and B for CSTR on the concentration space CA, CB. These solutions are known as CSTR locus. So you get discrete values corresponding to values of space time, tau chosen.

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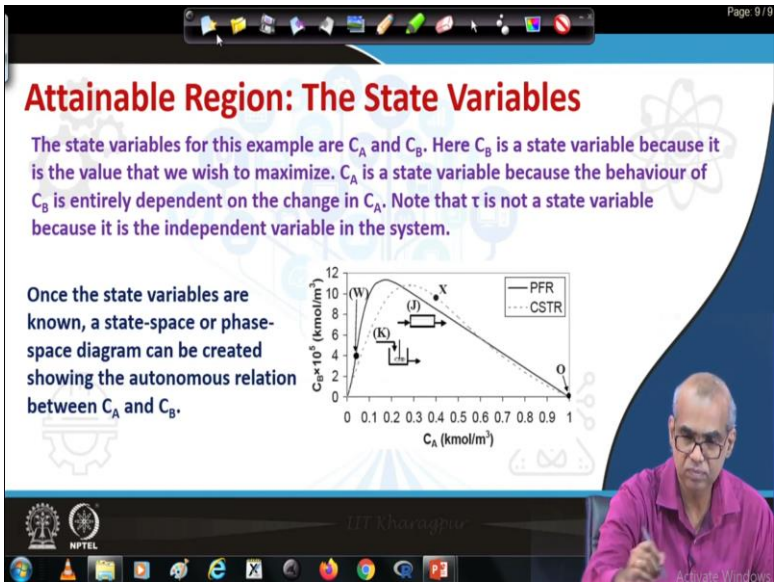

So after talking about PFR and CSTR as fundamental processes, let us now choose what will be the state variables for this system. The CB that which represents concentration of B is obvious state variable because this is the value you want to maximize. The concentration of A is also a state variable because the behavior of concentration of B is entirely dependent on the change in concentration of A.

So CA and CB are my chosen state variables. Note that tau is not a state variable, but this is an independent variable for the system. So once you have chosen the state variables we can draw the phase space diagram that means the concentration space diagram CA versus CB, and we have

plotted the PFR trajectory and also the CSTR locus which is shown as dotted line. So the trajectory shown by the continuous line represents the PFR trajectory in the figure and the trajectory shown by the dotted line represents the CSTR locus in this CA, CB figure.

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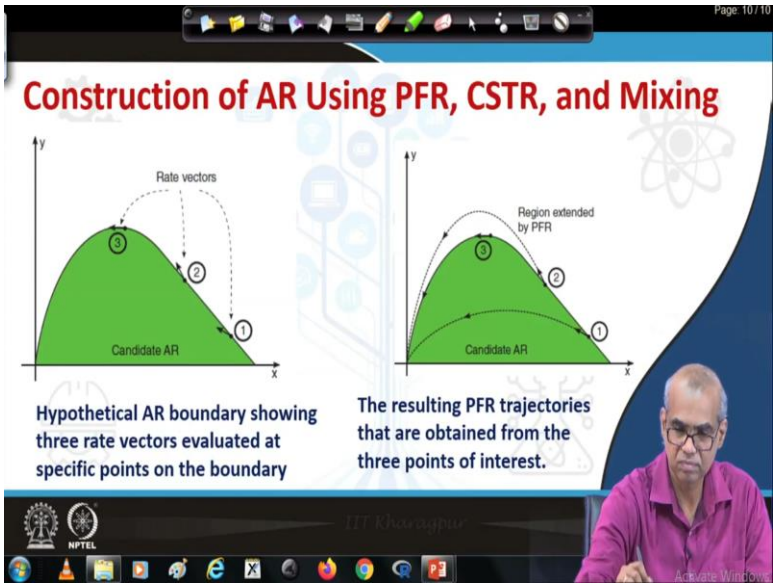

Now look at this left hand side figure first. This represents a hypothetical attainable region boundary and three rate vectors evaluated at specific points in the boundary are shown. 1, 2 and 3. So concentrate on the three rate vectors indicated by 1, 2 and 3. Now if we draw the PFR trajectories, we get the trajectories as this from 1, this from 2 and this one from 3. So clearly you see that the rate vector at point 2, which is pointing outside this shaded region or the previous candidate attainable region, extends the region. So the PFR trajectory drawn from point 2 extends that attainable region.

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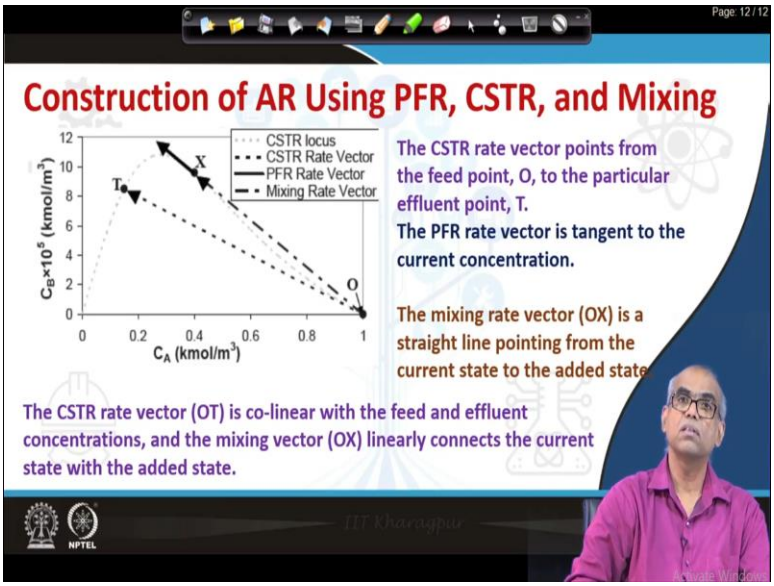

So we will look at the possibility of extending region by not only the mixing process but also by application of PFR trajectory. Now in this figure the CSTR rate vectors are shown as OT which points from the fit point O to a given effluent point T. Note that this dotted trajectory represents a CSTR locus. So point T represents an effluent stream coming out of a CSTR, O represents feed point.

So this CSTR rate vector OT points from the feed point O to the particular effluent point T. In just the previous slide we show that the rate vector for the PFR trajectory is tangent to the current state. So this represents a PFR rate vector. So this is tangent to the current state that means concentration. Note that the CSL locus here; it is a non-convex region, so this can be expanded by mixing.

So the mixing vector OX expands the CSTR trajectory or CSTR locus. The mixing vector OX represents a straight line pointing from the current state to the added state. So, from O to X the straight line are represents the mixing rate vector. The CSTR rate vector OT is collinear with the feed and effluent concentrations and the mixing vector OX linearly connects the current state with the added state.

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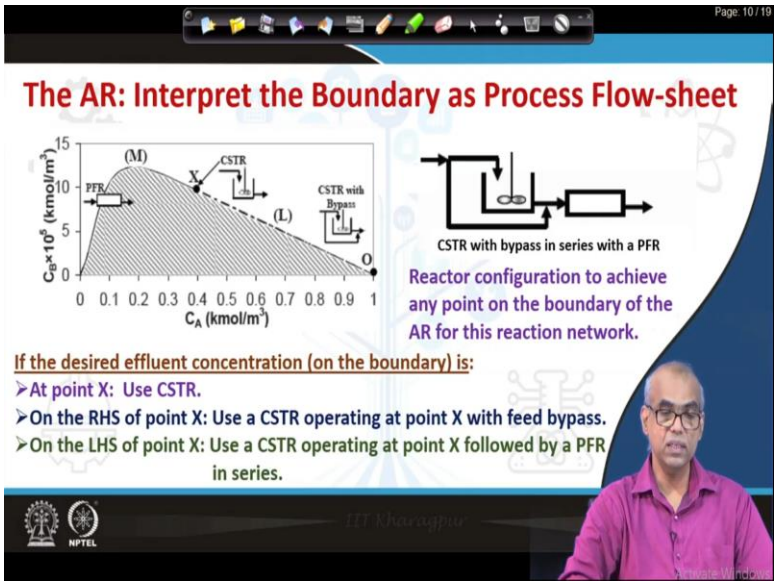

So we can extend the CSTR trajectory by mixing. So again consider the two trajectories the one represented by continuous line is from PFR which is given name J here and this boundary represented by K is CSTR locus. So consider the CSTR locus K, the straight line are OX correcting point X with the feed point O represents the mixing line and these extends the region. So L, line L represents this mixing.

So to achieve any concentration on line L we can mix the outlet of the CSTR operating at point X with the feed point represented by O. So any point on L which will represent the concentration of a mixture can be obtained by linearly combining the state at X which is nothing but effluent stream, from CSTR with the pure feed represented by point O. Thus any point on this line L corresponds to a CSTR with a bypass.

So this bypass is for mixing the feed with the effluent state. The Lever Arm Rule can be used to determine the percentage of each stream that needs to be mixed.

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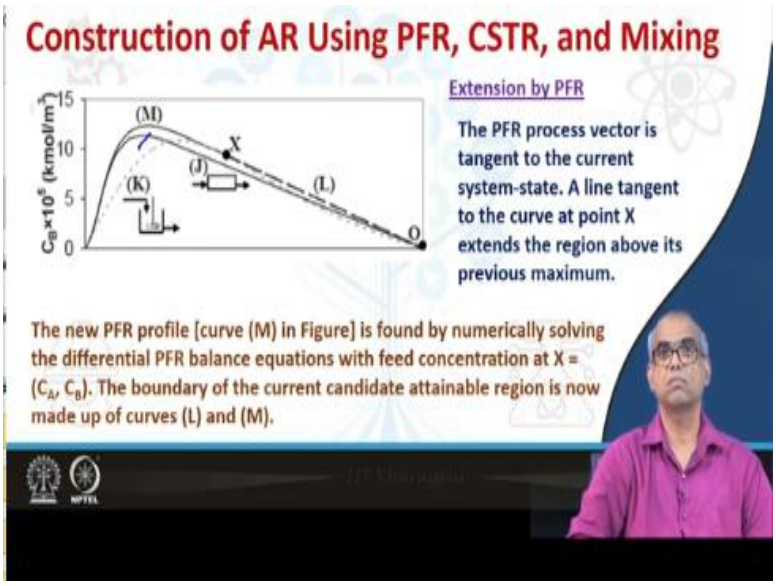

Now let us see whether we can further extend the region by PFR trajectory. The PFR process vector is tangent to the current system step. So a line tangent to the curve at point X extends the region above its previous maximum. Note that this was the previous Trajectory. Now from point X if I draw another PFR trajectory it extends the region above the previous maximum. This is possible because PFR process vector is tangent to the current system state at X.

So I can draw a PFR trajectory from point X and extend the previous candidate attainable region. So how do you get this new PFR profiler PFR trajectory, which is represented by curve M in the figure. This can be found numerically by solving the differential equations for the PFR with the initial condition as given by point X. So point X that represents concentration of A and concentration of B which comes out of the CSTR.

So they are the CSTR effluent concentrations. So to obtain the trajectory indicated by curve M, we have to numerically solve the ordinary differential equation that represents PFR with initial conditions given by point X. So now the current boundary of the candidate attainable region is given by the curves L and M. Now if there is no scope for further expansions of that attainable region or the candidate attainable region, we have obtained our desired attainable region.

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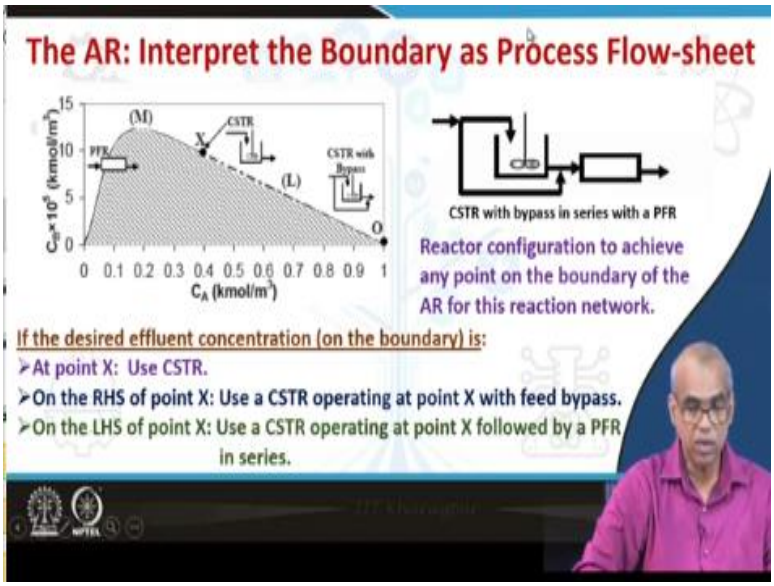

So the construction of attainable region is complete once it has been determined that no other processes can extend the region. The shaded region in the figure shows the entire attainable region for this particular reaction network, that means that van de Vusse reaction scheme. So the boundary of that attainable region is made up of curves L and M. Note that the region is convex it is clear that the mixing cannot extend the region.

At this point all the rate vectors on the boundary are either tangent to the boundary or point into the region. Any point within the boundary represents an attainable reactor effluent given a feed point at O. So given the feed point as indicated by point O any point within the serial shaded region is attainable. So now we are obtained our attainable region for the process. Now look at point X, point X represents a CSTR. Point O is my feed point; any point on the line L or OX represents a CSTR with a bypass.

So the point X represents a CSTR, so if you have to get the concentrations of B that is given by point X use a CSTR and any point on the right hand side of point X can be achieved by using a CSTR operating at point X with a feed bypass. What percentage of it bypass you have to use can be obtained following lever arm rule. Any point on the left hand side of point X can be obtained by using CSTR operating at point X, followed by a PFR in series.

So any point on the left of point X can be obtained by connecting a PFR in series with the CSTR,

so CSTA followed by a PFR in series. So this CSTR with bypass in series with a PFR is the reactor configuration to achieve any point on the boundary of the attainable region for this scheme. CSTR with bypass in series with a plug flow reactor can be used to achieve any point on the boundary of the attainable region for this reaction network. So you obtained our reactor network structure that needs to be used to obtain any point on the boundary of the attainable region.

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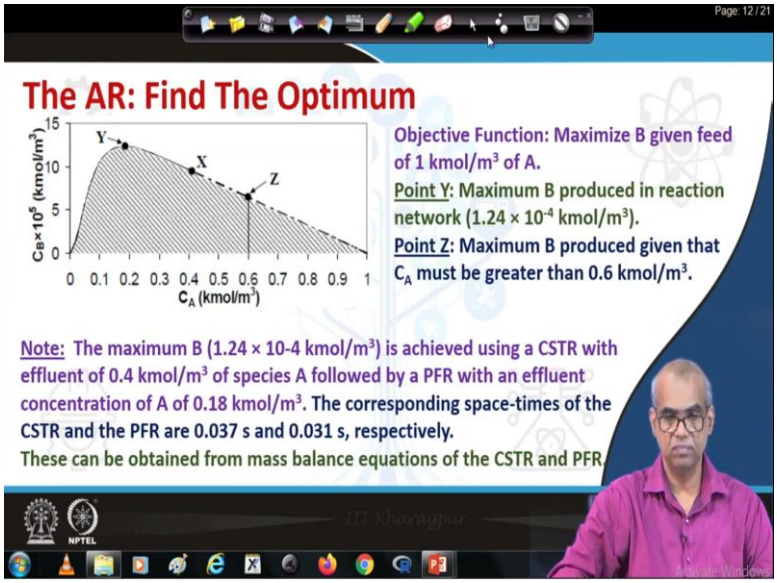
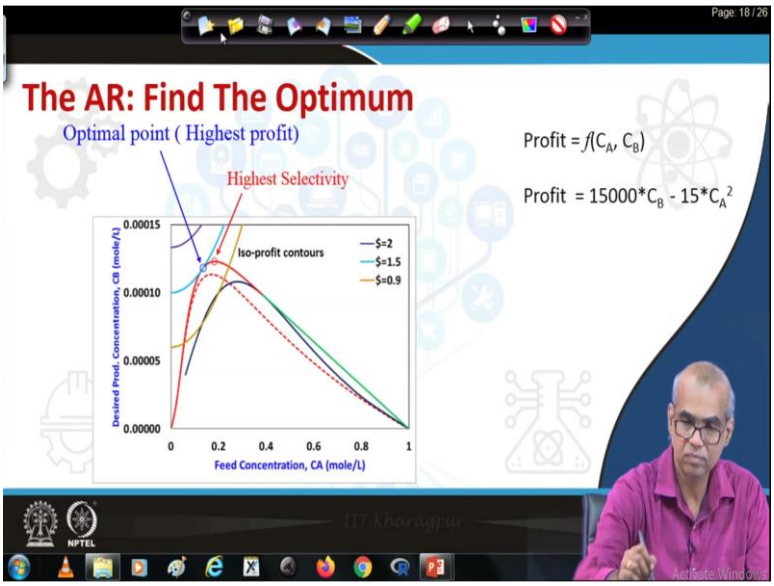


Now let us look at optimization part of it my objective is to maximize B given feed of 1 kilo mole per meter cube of a in this particular case. Clearly from the figure we see that point Y represents maximum B produced in the reaction network. Now if I ask the following question what will be the maximum amount of B produced given that CA must be greater than 0.6 kilo mole per meter cube. So 0.6 is the bound on concentration of A.

So that is represented by point Z which corresponds to CA equal to 0.6. Now again concentrate on point Y which represents maximum concentration of B for this reaction scheme starting with feed 1 kilo mole per meter cube. How do you obtain CA, how do you obtain CB the maximum CB? See this will be achieved using CSTR effluent at point X so which is 0.4 kilo mole per meter cube of species A, followed by a PFR with effluent concentration of 0.18 kilo mole per meter cube of A.

Note that Y represents a point on the left hand side of X, so this can be achieved by CSTR operating at point X followed by PFR. How do you find out the corresponding space time of CSTR and PFR? They can be obtained from the mass balance equations of CSTR and PFR. **(Refer Slide Time: 31:15)**



Now some more point about the optimization. Let us say instead of having the objective of maximizing B which represents higher selectivity. I have a profit expression, which is a function of concentration of A and B. For example, let us say I have this equation. So how do I find out the optimum point? So what I do is, I draw the profit contours, so these are my profit contours. So what does what do they mean they are isoprophic contours means, any point on these lines represent the same profit.

For example this corresponds to profit 2, this is 1.5 and this is 0.9 so on and so forth. So the profit increases along this. So obviously who are interested in finding out the point in this boundary of the air that passes through a contour, which is as further away as possible in this direction because as the direction of maximum value of profit. So that is clearly indicated by this point.

So that is the optimal point when my objective function is a function of A and B. For example in this particular case this. Whereas the highest selectivity is not the same optimal point, note that the highest selectivity is the maximum on this attainable region curve. But if I consider the profit

contour that passes through this point this will have lower profit value than this because it is increasing in this direction. So this way such diagrams can also be used to analyze different types of objective functions.

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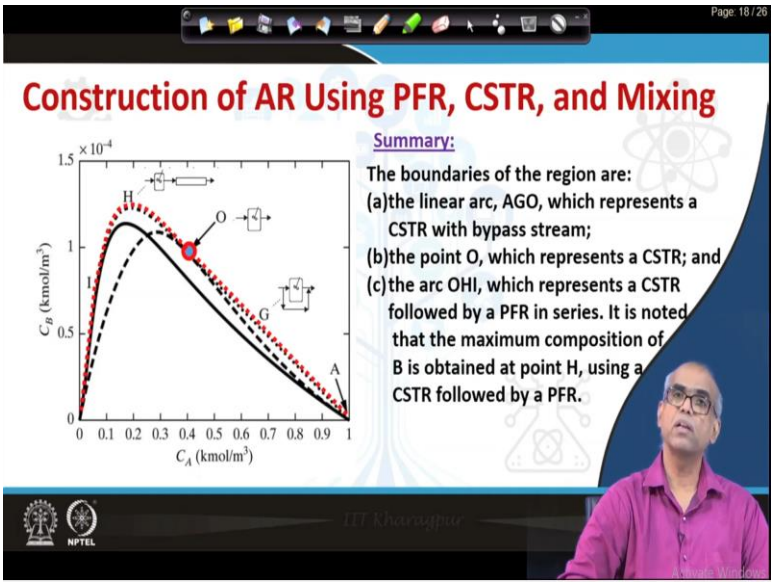

So this is the summary we start with we can start with the PFR the look at the CSTR whether this expense the region or not draw the linear herbs and then find out the scope for further extending that enable region using PFR trajectory, where no further expansion is possible, either through PFR at trajectory or through mixing you have obtained your attainable region.

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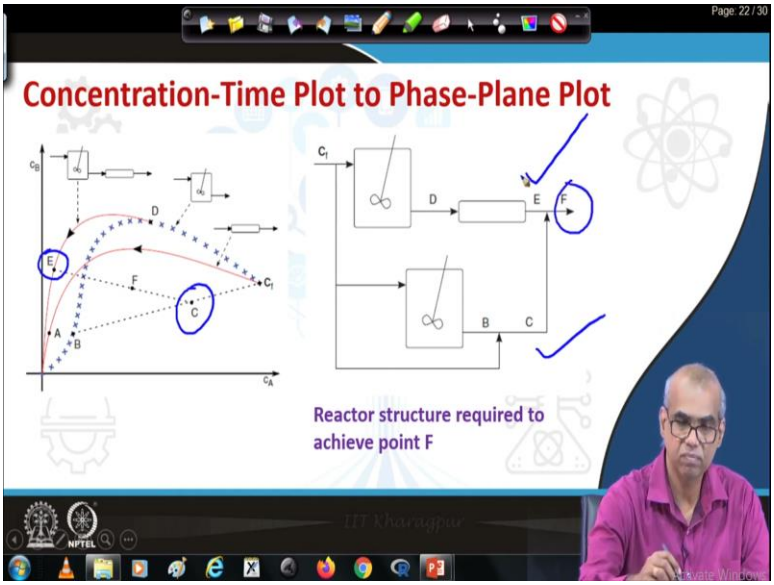

Now let us ask one question, suppose the CSTR and PFR equations are solved for two

dimensional system involving components A and B and the plot in the figure is generated. So this is the figure we have generated, now what reactor structure would be required to achieve point A, point C and point F. Note that point a falls on this PFR trajectory, point C is this and point F is this.

Point C and point F is lying within the region does not fall any trajectory that as shown in this figure. So how do you get this, since point A is directly lying on this PFR trajectory I can use this PFR to obtain point A. What about point C? Point C is lying here, look at point B which lies on the CSTR locus and if I join the feed point with point B, I can obtain point C. So to obtain point B, I need a CSTR and to obtain point C, I need to mix the effluent stream with the feed given by CF. So a CSTR with a bypass is required to obtain point C.

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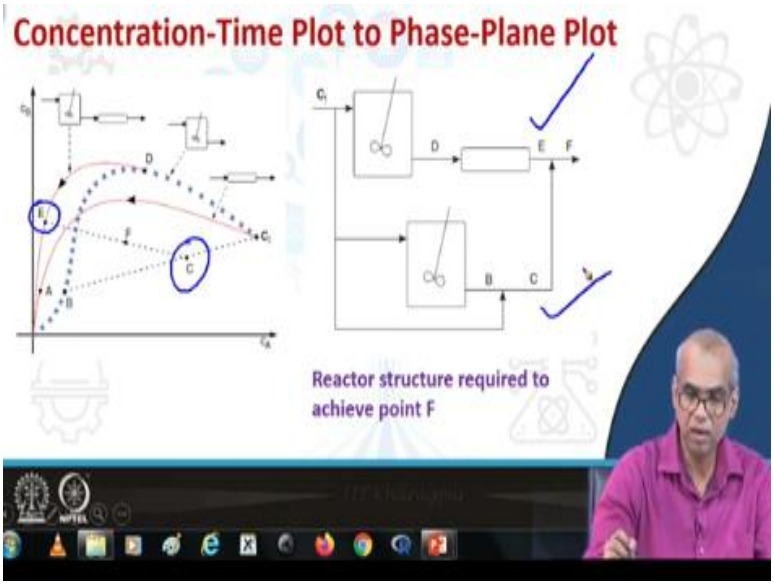

Finally to obtain point F, I have to make point C and point E. Point E is lying on this trajectory which can be obtained by CSTR followed by PFR in series. So you obtain that point E first and then point C can be obtained by CSTR with bypass, CSTR and the bypass to mix the effluent with the feed stream. So this together they will give you point F. So all you have to do is you have to first get E and then you get C with CSTR and bypass and then there being mixed to obtain point F.

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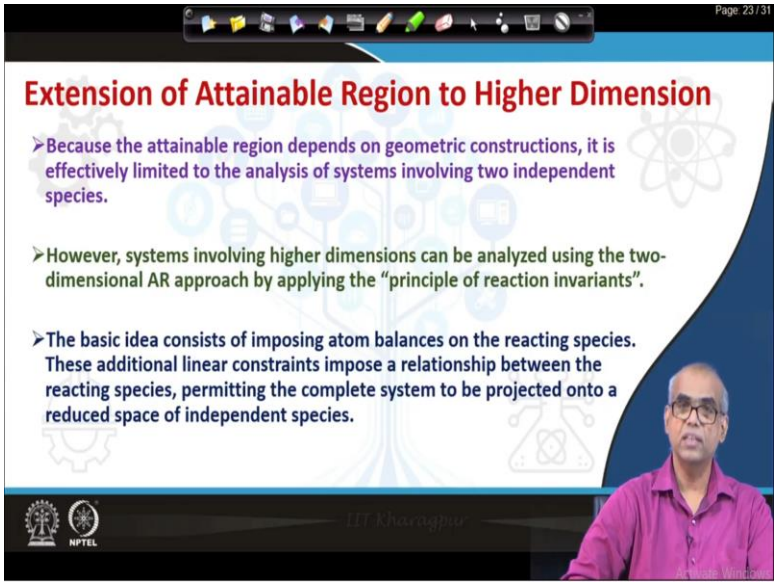

So we will stop this discussion with the comment on how to apply this on higher dimension because the attainable region depends on geometric constructions, it is effectively limited to the analysis of systems involving two independent species. However systems involving higher dimensions can be analyzed using the two dimensional attainable region approach by applying the principle of reaction invariance.

The basic idea consists of imposing atom balances on the reacting spaces, these additional linear constants impose a relationship between the reacting species permitting the complete system. To be projected onto a reduced space of independent spaces. So the purpose of telling this is just to tell you that it is also applicable to higher dimensions. It is the attainable region is a geometric construction.

So it is best analyzed on two dimensions, but it is possible to extend it to higher dimensions using the principle of reaction invariants. With this we stop our discussions here.