Multiphase Flows: Analytical Solutions and Stability Analysis
Prof. S. Pushpavanam
Department of Chemical Engineering
Indian Institute of Technology – Madras

Lecture – 22
Stability of a Reaction-Diffusion System contd.

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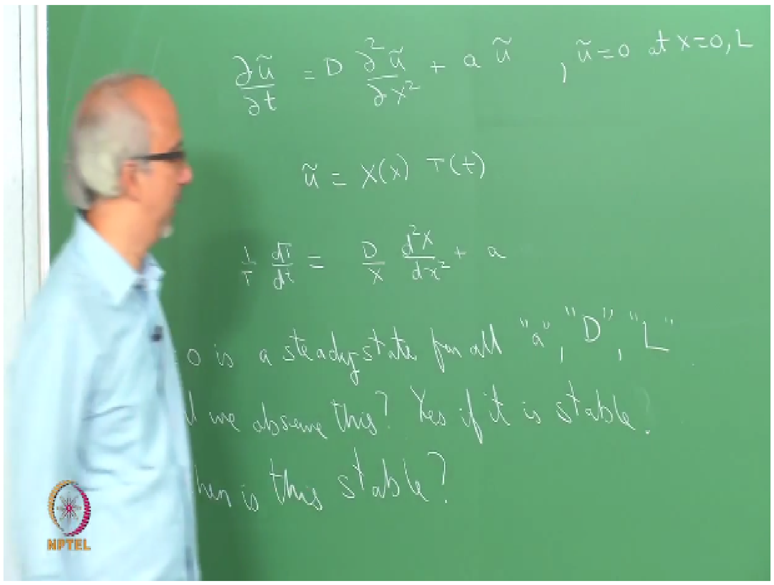

Welcome to the lecture where we are discussing the stability of the solution to reaction-diffusion equation, okay and what we did till the last time was we found a solution which was spatially uniform, which was basically saying that the steady state was 0 for all values of the parameter, okay. We decided we will ask the question whether such a solution is stable because if stable that means you will actually observe it. If it is not stable that means you are not going to observe it, okay.

So, that was a question which we wanted to find out the answer to and in the process what we did was we found the steady state, we did the linearisation and this was the linearise equation. Now, what you have to remember is that uss=0 is a steady state for all values of a, d and l. It is always a steady state, okay that is something which I want you to remember now because recall that uss=0 is steady state for all a, a is something like a reaction rate constant, okay, D is diffusion coefficient and L is the length of the thickness of the catalyst.

So, these are the 3 physical parameters, no matter what you take for all combinations, this is always possible steady state, okay. Now, the question is will we observe this, that is the question and answer is yes if it is stable, that is the answer but the question is when it is stable and that is what we are trying to find out, okay. So, when is this stable, that is the next question and that is what I am trying to out now when is this particular steady state stable.

So, in the process what we have to do is we have to solve this linear equation which is subject to homogenous boundary conditions. The boundary conditions are u tilde=0 at x=0 and L, okay. Since it is a linear equation, we decided to seek a solution in the form of variable separable form and we substituted this here and then we get this equation; and with a little bit of rearrangement, you will find that the left hand side is the function of time.

The right hand side is a function only of x and the only way these 2 function can be equal is if both of these are equal to a constant. So, what I am going to do now, since it is a constant, there are basically 3 possibilities. The constant can be positive; it could be 0 or it could be negative.

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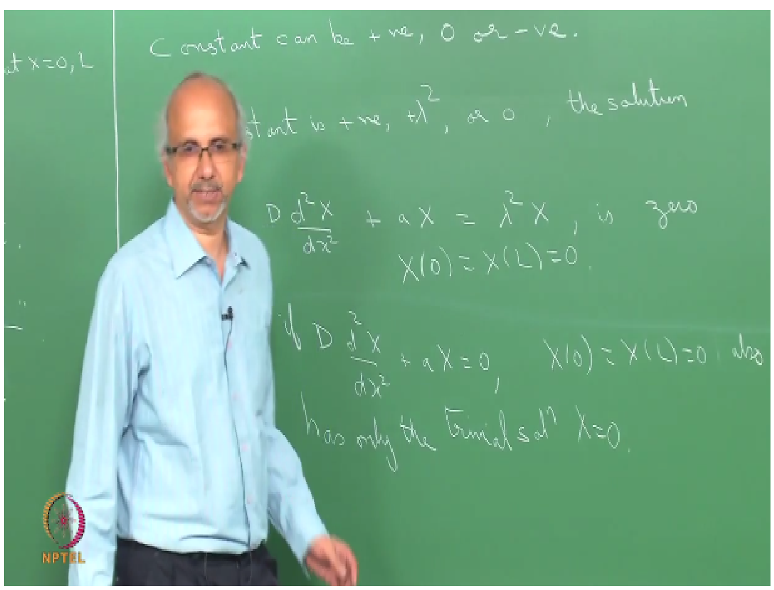

So, this constant can be positive, 0 or negative, right. What we are looking is a non-zero solution to this differential equation. I mean 0 is a solution always but if you get 0 as a solution that means why, your perturbation is 0 but what we want is given a particular perturbation as time goes to infinity, we want to find out how the system is going to behave.

So, we are interested in finding out a non-zero solution. So, I am going to claim and this is something you people have to verify that if this constant is positive or if this constant is 0, the solution to this equation, the second order equation x is going to be 0, okay. What I am saying is if this constant is positive, let us say plus lambda square are 0, I am saying plus lambda square, lambda square just to tell you it is positive and a plus sign in front.

There is no way this guy can be negative or 0, the solution to this equation is d square x/d x square*D+ax=lambda square x is 0 where it is subject to the boundary condition, x of 0=x of l=0. So, how do I get these boundary conditions on x if these come from the boundary conditions on u, u is 0 as the 2 ends, so the only way u can be 0 at the 2 ends is if x is 0 at the 2 ends.

So, x has to be 0 at the 2 ends and then if x is 0 at the 2 ends, I am saying if you solve this equation, the solution is 0 if you have plus lambda square. If you have d square x/dx square + x=0 subject to x of 0=x of l=0 also has only the trivial solution x=0, you understand. I want you to verify this. You can just proceed, do the algebra, find the solution to this, put the boundary conditions and see if you can get non-zero solution, okay.

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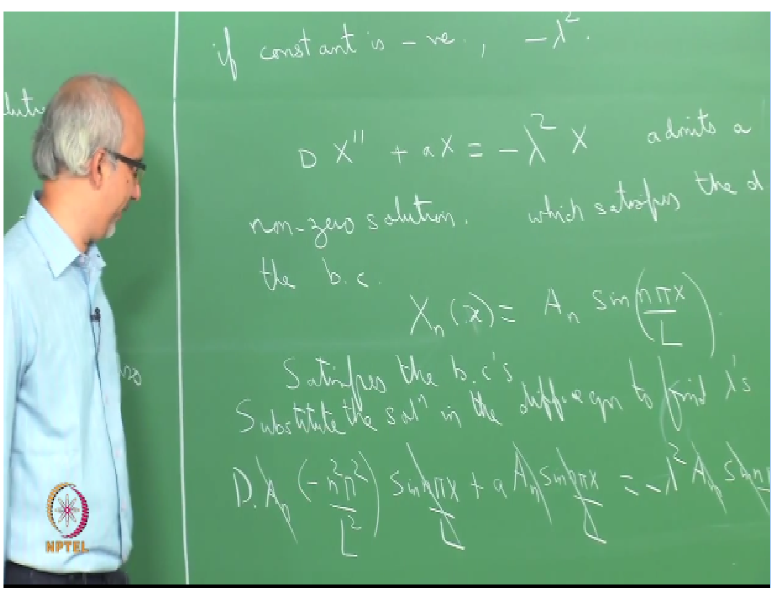

However, if the constant is negative and I am going to indicate that as minus lambda square, then this equation dx double prime for the second derivative plus ax=-lambda square xa admits a non-zero solution. This is basically what you have done all along in your separation of variable solution. In your separation of variable solution, you have assumed this constant be equal to minus lambda square and you proceed it.

So, the reason why you assume this minus lambda square is because that is thing which gives you the non-zero solution and that is what you want. If you assume plus lambda square and you will find that it gives you only the 0 solution, we assume 0 we get only the 0 solution. So, I am just trying to justify why I am putting minus lambda square, okay, which satisfies both the differential equation and the boundary condition.

So, what is the non-zero solution which will satisfy the differential equation and the boundary condition. I am going to claim and this is something which you people have done whenever you have done the separation of variables. For example, sin n pi x/L. This is in fact you will have sin as well as cosine but because of the boundary conditions, you can prove that the cosine term does not exist, only the sin term exists, okay.

Sin n pi x/L satisfies the boundary conditions, does everybody understand this, sin n pi x/L. See I am saying this solution Xn of x, this satisfies the boundary conditions, okay and you can possibly do this in a slightly more formal way but since I have done this problem so many times and since you have also done this problem in calculus, you should be able to figure out. I am just jumping a few steps. Although it satisfies the boundary conditions, I have to make sure that it satisfies the differential equation, right.

What I do not know yet is the lambda square. I do not know what lambda square is, okay. So, I am going to substitute this here and find out that the lambda square what it is in terms of this n pi and the other stuff, that is the plan. So, to find lambda what I will do is I will just substitute the second derivative which gives me substitute, the solution in the differential equation to find the lambdas, okay. So, let us do that.

What do we get, you have the d, you have the An and when you differentiate it 2 times you get minus n square pi square/l square*sin n pi x/L +a*An sin n pi x/L =-lambda square An sin n pi x/L. So, this is a typical Eigenvalue problem which you people have come across before, okay and you know that the solution is sin n pi x/L. I am just exploiting the knowledge which you already have in proposing the solution. Only thing is normally your Eigenvalue performance will not have this ax term.

Now, there is an extra ax term here. You have solved problems where you have x double prime=-lambda square. So, all I am doing now is I am going to realize that An sin n pi x exists everywhere and so this equation because I am interested in a non-zero value, An sin n pi x is not 0, I can cancel it off.

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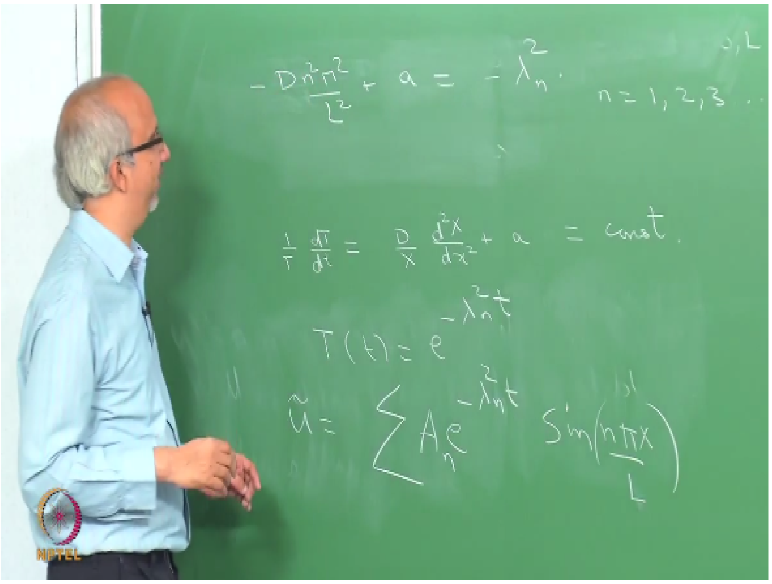

What I get is the diffuse coefficient*n square pi square/L square +a=-lambda square, okay. So, basically what I am trying to tell you is that the lambda square. Remember what is n, n goes from 1, 2, 3…. etc., it is an integer, okay. Correspond to different values of n, I will have different lambdas, so I am going to put a subscript n here. Now, I put this constant as minus lambda square. So, what will be the solution for T. The T of t is going to be of the form e power minus lambda n square t, okay, that will be the solution for T.

So, I am saying that u tilde is, if you remember your separation of variables is going to be summed over all these ends and is going to be of the form e power minus lambda n square t*An sin n pi x/L. So, this is basically how the perturbation is going to change with both space and time. Now, this is the mathematical solution which we have obtained but I want you to think of this thing in physical terms. When you are giving a perturbation or a disturbance to the solution, the solution is us=0, you are giving some perturbation. What happens because of this perturbation. In some points, instead of 0 you have a non-zero value for the u, okay.

The perturbation is the deviation of the actual value from the steady state. So, we can do is we can thing of the perturbation at time t=0 which is when I am starting the experiment as going to be some function of x as a function of x in the interval from 0 to L. Now, if you were to extend this function of x periodically, okay, you can basically represent this function of x in the form of 4ier sine series. So, what we have done is think of an arbitrary perturbation.

If you had expanded this in the form of 4ier sine series, the time t=0, these coefficients would basically tell you how this particular disturbance is resolved along these components. So, this is just like resolving a vector in terms of some basis of vector. You take an arbitrary vector, you can write it in terms of some basis e1, e2, e3, 10001, 10001, okay. So, therefore you should look at this is, look at some function which is your perturbation at time t=0 is resolved in terms of these Eigen functions, okay, the sin.

Now, the question is our interest is to find out how do things behave as time t goes to infinity. Clearly that is going to be decided by the lambda n square, okay. There is already a negative sign here, so if the lambda n square was negative, then this negative and negative would be positive and you would have the thing blowing up, becoming unstable. If lambda n square is positive, then it is going to decay, okay.

So, let me just summarise whatever I have said and then how we calculate lambda n square that basically depends upon the diffusion coefficient, the geometry, the red constant, that is what you want, okay. So, that is basically the link in the loop which you are trying to close.

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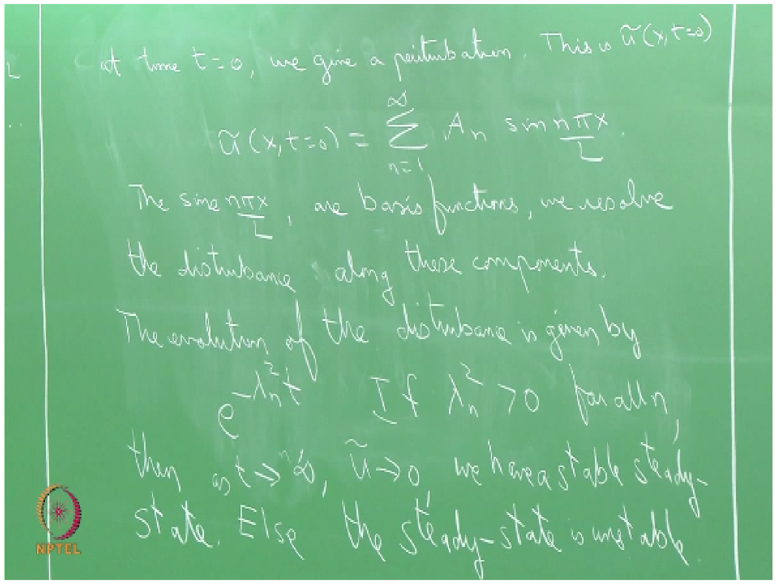

So, at time t=0, we give a perturbation and this is u tilde of x, t=0 okay, and what I am saying is when I write u tilde of x, t=0, my solution is An sin n pi x/L. I am just saying that what we are doing is this is a function of x and resolving this function of x in terms of the basis function, just like you resolve a vector in terms of basis vector, okay. So, this is the sin n pi x/L are by basis function and we resolve the disturbance along these components, okay.

That is the way I would want you to look at this physically, mathematically of course you got the solution, okay. So, how does each of this. Like for example, in the finite dimensional problem you had a vector disturbance, you had 2 Eigen vectors and you wrote it in terms of 2 Eigen vectors. Instead of 2 Eigen vectors, I have an infinite (()) (18:33) where this summation is going from n=1 to infinity.

So, from what was the finite dimensional problem, we have moved to an infinite dimensional problem, okay. So, this is our basis function, okay and the evolution of the disturbance is given by e power –lambda n square t, okay, the time dependency and what we are interested in is as t tends to infinity, the guy has to go to 0. So, lambda n square is positive for all n, then as t tends to infinity u tilde tends to 0 and we have a stable steady state, okay, else the steady state is unstable.

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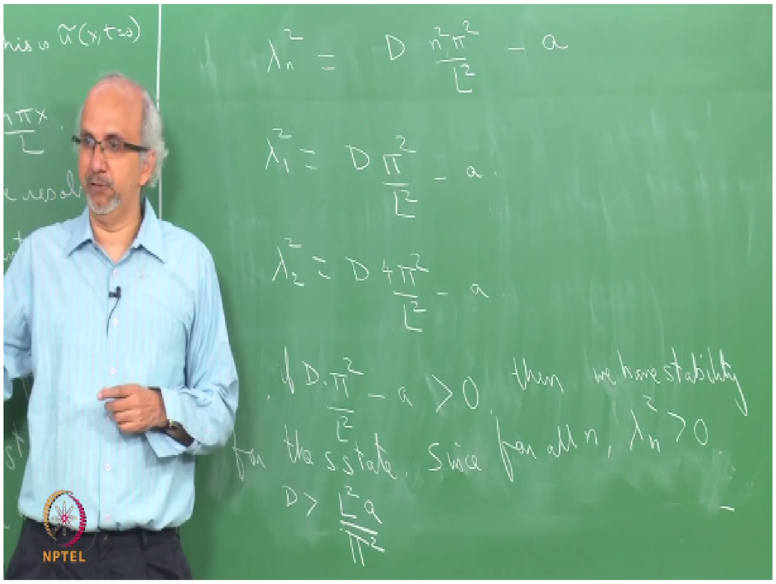

So, now remember lambda n square=D times n square pi square/L square-a, okay. So, I have different Eigenvalues. Lambda 1 square=D times pi square/L square-a. Lambda 2 square is and so on and so forth, right. So, now what do I want. If lambda n square is positive for all n, then we have a stable steady state, okay. So, if D pi square/L square-a<0, that means this guy is positive. I do not like this. I am doing something wrong. Have I done something wrong here.

Now, I want lambdas to be positive for stability, right. I want lambda square to be positive. If this is > 0, then we have stability for the steady state. Why, because this guy is positive where all the other fellows are positive. The first one is positive, so when I take 4 pi square. If D pi square/L square-a is positive, then D4 pi square/L square-a is positive, 9 pi square/L square*D-a is positive and so on and so forth, okay, because I was increasing this guy the positive fellow.

This is of course the positive domain, diffusion coefficient number is positive, okay. So, this guy is positive and it keeps on increasing. Then, we have stability for the study. Since for all n, lambda n square is > 0, okay, which means D>L square a/pi square and that is the threshold value, that is the critical value of the diffusion coefficient. If it was for a given slab, for a given reaction which is decided by the rate constant a, for a given reaction which decides a, for a given slab which decides what the thickness is L, geometry is fixed, kinetic is fixed and diffusion coefficient is only other parameter.

If the diffusion coefficient is greater than this number, okay, then you have a stable solution for uss=0 and that is basically what we said earlier. Remember if the diffusion coefficient is very large, then you would have any concentration variation which is present in the slab will get smeared out because diffusion will flatten it, because that is what diffusion does. If you have a room where there is concentration gradient and you just leave it, diffusion is going to make it all equal, okay.

If the diffusion is greater than this critical value, you have a stable steady state. If the diffusion coefficient is less than this critical value, then this guy is going to be negative. These guys we do not (()) (25:16). These guys could be positive, negative. The first guy to become negative is going to be this. The first lambda n square which becomes negative will correspond to n=1. This is the first guy; all these guys will be positive.

So, this guy will become negative first, then this guy will become negative as you keep lowering D, okay. So, the first guy to become negative will be this guy. If this becomes negative, then remember the solution is going to grow exponentially, okay. So, that is basically the onset of instability which means uss=0 is not going to be observed if the diffusion coefficient is lower than this value.

If the diffusion coefficient is less, you will have a non-zero solution, you will have some function. You get some idea about how that function is by looking at the corresponding value of Eigen function here, sin n pi x/L. Sin n pi x/L tells you how the spatial variation is going to be of the non-zero solution. So, the non-zero solution that you are going to get is going to be of the form corresponding to n=1 is going to be of the form sin pi x/L.

It is going to go to 0 as the 2 ends and it is going to have one kind of hump in the middle, okay. So, that is basically what the information is which is present in the Eigen function.

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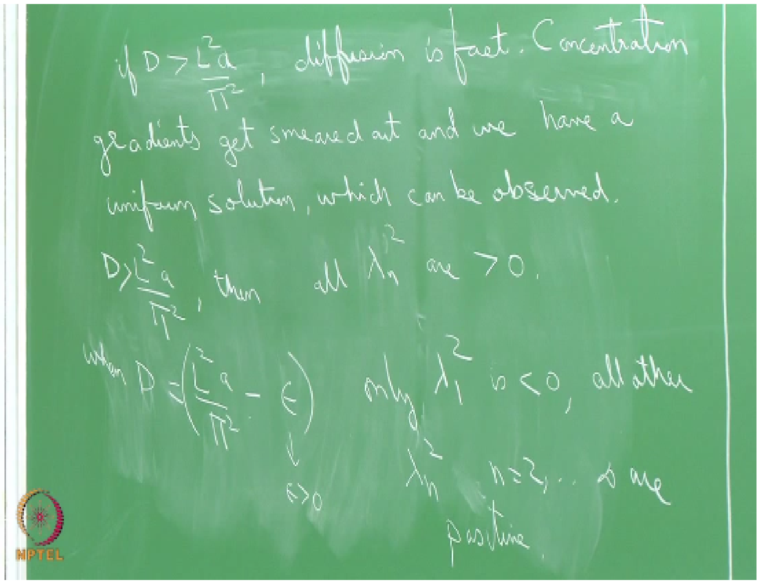

So, now I am just going to write this thing down. So, if D>L square a/pi square, diffusion is fast that means concentration get smeared out and we have a uniform solution which can be observed and that is stable, okay. If D>L square a/pi square, then all the lambda n square>0 and therefore the solution is stable. When, D<L square a/pi square, slightly less than, okay. I should say is equal to L square a/pi square-epsilon where epsilon is positive and small. So, slightly less than this, then what happens, only lambda 1 square is negative.

All other lambda n square, that is for n=2 to infinitely are positive, okay. When slightly less, only lambda 1 square will be negative. Lambda 2 square is multiplied by 4, so that guy will still be positive, all others are positive. So, what that means is supposing you have a disturbance and you resolve it in terms of sin pi x/L, sin 2 pi x/L, sin 4 pi x/L, the thing which is going to grow is the one corresponding to sin pi x/L, corresponding to n=1, that is the only mode which is going to grow.

The modes corresponding to n=2, 3, 4, 5, they are going to decay. As a result, what we are going to observe in your system is going to be the solution which corresponds to sin pi x/L, okay. So, that is the insight which you are getting.

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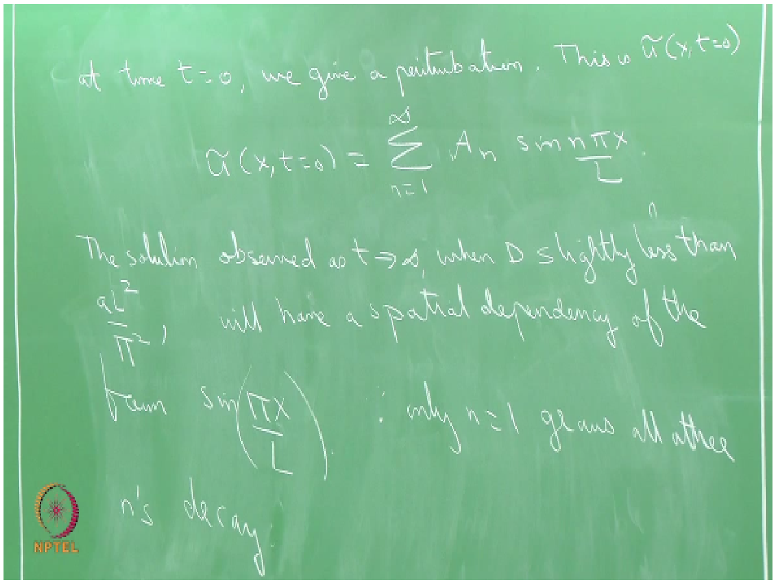

The solution observed as t tends to infinity when D is slightly < a L square/pi square will have a spatial dependency of the form sin pi x/L. Because only corresponding to n=1 is going to grow, okay. Since only n=1 grows, all other n's decay, okay. So, what this means is you will get something like solution for you which has got some kind of non-zero value inside, may be the single maxima, okay. So, I think this is just to illustrate to you that you have a critical value.

So, there are 2 processes which are taking place; one is a reaction process and one is a diffusion process, okay. If the diffusion process is slow, if the diffusion coefficient is very low, then you will have a non-zero solution, but if the diffusion is very fast, then you have a spatial homogeneity and our solution is stable, okay, that is what physically you expect. But what the theory, what the mathematics allows you to do is try to get you what this critical value is of the diffusion coefficient, okay.

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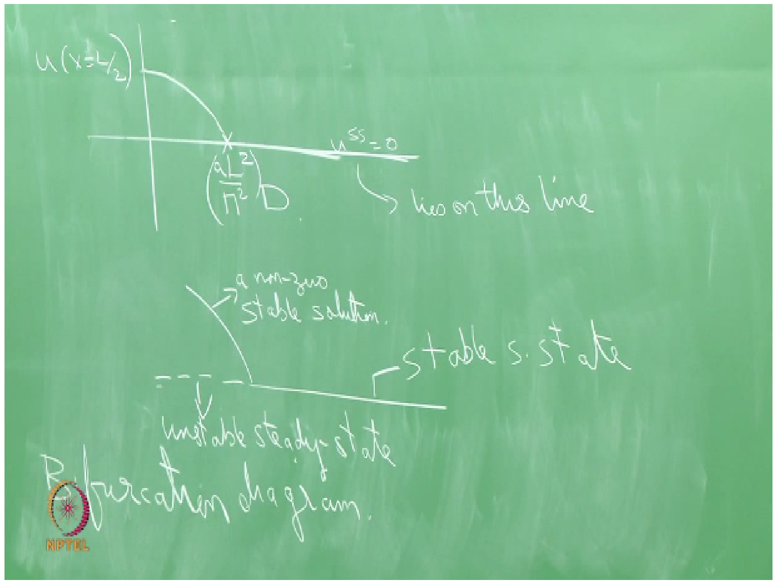

So, what this means is if you actually have a plot. So, if we made a plot of, let us say, u versus D, okay and let us say we are plotting u at the centre point, u at x=L/2 in a steady state solution. As a function of D, what do I have. So, high values of D, I know that 0 is my solution which is stable, what I am going to observe is 0, okay. So, this is the value of a solution that I am going to observe. This is uss=0. So, uss=0 is along this line. My uss=0 means everywhere it is 0, therefore at the centre point also it is going to be 0, okay.

So, what I am doing here. I am trying to represent how the steady state depends upon the parameter D. So, the point is uss=0 lies on this line and this is true for all D, all the values of diffusion coefficient. Of course, we do not want to go to negative diffusion coefficient because that does not make sense. The point I am trying to make here is this guy, this is let us say my critical value. What is my critical value?

What is my critical value a L square/pi square and that is the number which I can calculate and I am just putting a plot there. I am saying when D is less than this, I am not going to observe this, whereas I will get some other non-zero value inside my (()) (34:18) slab and I want to represent that non-zero value. So, I am just taking the value at a particular point. So, let us say it is going to be positive value, it is going to be some non-zero value which may be keep on increasing.

So, as I keep decreasing the diffusion coefficient, the magnitude of the concentration at the centre of the pallet is going to keep on increasing. The farther I go away from this, the more is going to be the value at the centre. So, what we normally do to represent this kind of pictures, we want to represent the stability information also on this kind of a picture, okay. So, the way this is classically done is this.

This is just to tell that whenever I have a solid line, that represents a stable steady state solution. When I have a dash line, I have an unstable steady state solution. So, this is a stable steady state, okay. This is an unstable steady state, okay. So, when D is sufficiently large, I get the stable steady stable. I can actually observe it experimentally. But if you keep on decreasing the diffusion coefficient, calculation tells you that the steady state is unstable, now what does it mean.

Whether it means that catheter is going to vaporise or does it means something else is going to happen. Nothing crazy like that is going to happen, right. So, what is going to happen is we are going to have a non-zero solution, that means this non-zero solution now is going to be the steady solution because that is what we are going to actually observe experimentally. So, that is reason I have drawn this by solid line. This is a non-zero stable solution.

I am telling you that this particular branch which I am getting is another solution, okay and if you want we can calculate the other solution by doing a finite difference scheme for the partial differential equation or for the OD equation you can just solve it by using some numerical method, because it is a non-linear equation and you can get this branch, but this is also a steady solution but this will be observed only when the diffusion coefficient is sufficiently low.

If the diffusion coefficient is sufficiently large, this guy will not exist. This guy will collapse to u=0. So, this kind of a diagram where I am trying to represent the behaviour of a particular system or a solution versus a parameter is called a bifurcation diagram, okay. What I have drawn here is actually a bifurcation diagram. So, this is bifurcation diagram, okay.

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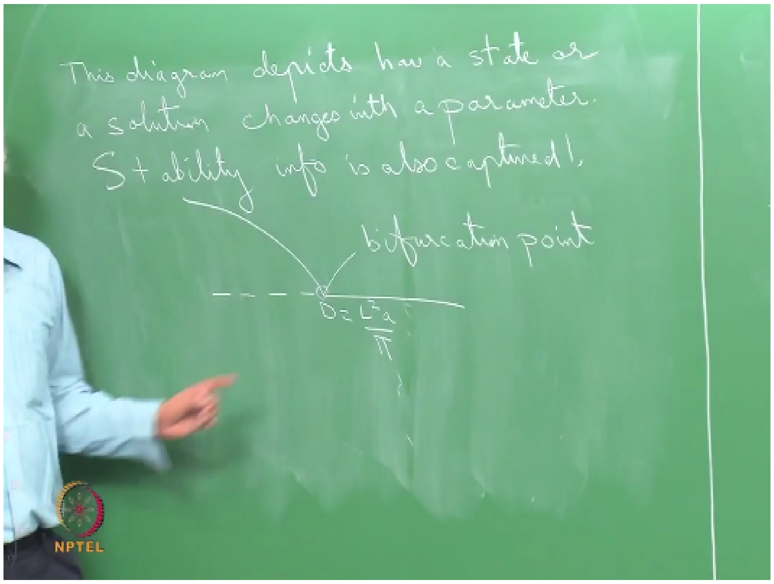

What does a bifurcation diagram do? This diagram depicts how a state or a solution changes with a parameter and the stability information is also captured, and I am going to redraw that thing which I had drawn earlier and this is D=L square a/pi. This particular point where you have a change from one branch to another is called the bifurcation point. So, the bifurcation point is a point where a new solution branch is emerging.

So, I have this steady state solution which always exists, okay because you will put uss=0, it satisfies the equation always, no matter for all values of a, D and L. You, however, want to know if you can experimentally actually observe that steady state and that is where the question of stability comes in. Then, you do the linear stability analysis and then it tells you only if diffusion coefficient is sufficiently large more than this critical value, you will actually experimentally observe and this has been shown by a solid line.

For lower values of diffusion coefficient, I have this dash line. But what happens, I mean when diffusion coefficient is low, clearly there has to be some kind of reaction going on, something has to be happening in the pallet, right. So, there has to be some other solution which is going to be present in the system and that other solution is going to be of the form sin pi x/L and that is the linear stability analysis tells you.

So, you get a non-zero value for the concentration inside the pallet and this non-zero value I am just depicting in the form of this kind of parabola. Physically, I expect that farther I go away, the more is going to be the amplitude, correct. As I come closer, it should collapse to 0. So, as I go away, it should be more. So, I am drawing it in form of this kind of a parabola to tell you that this is the kind of a parabolic dependency this solution has, okay.

So, that is basically it as far as this particular problem is concerned, okay. I do not know if I have jumped too fast when I wrote down this Eigenvalue thing, but you can solve that linear equation for X in different ways, you will get the same conclusion, okay. If we get a different conclusion, then what you have done is wrong. If we came to conclusion, then what you have done is okay.

So, what we have seen is how varying a parameter, of course experimentally you cannot really be very diffusion coefficient that is a very difficult parameter for you to vary. The only way you can vary a diffusion coefficient is by either making the ports bigger or by changing the gas, but this is just to illustrate the concept. But maybe what we can do is think varying the length of the slab, okay. So, if the length is going to be sufficiently low, you will have spatially uniform solution, because the distance to which it has to diffuse is lower.

Thickness of the slab is very large, that means the diffusion resistance is high. So, you can just invert the problem and then say talk in terms of the thickness of the slab for which you want to get a uniform solution. So, this may have some implication, especially if you have a non-isothermal reactor where you may want to keep the temperature uniform for example, because you may not want to have the temperature go too high inside the catalyst, okay.

For other reasons, like may be undesired side reactions are taking place but the essential idea is when you do a linear (()) (42:01) analysis, what you can do is you can find these kind of transition points where a solution becomes unstable, a new solution is emerging and this will correspond to some basic change in the physics of the process.

Something which was dominating, diffusion which was faster has now become slower and that has basically what has caused and it is the relative rate of diffusion and reaction rate that we always have to look at, okay. So, we will stop with this for now and we will move on to a problem in fluid mechanics which is again going to be a partial differential equation but with system of equations and then we will solve and that particular problem that we will be looking at is the problem of natural conviction which is called the (()) (42:52) problem, that we will have only one fluid but it will have 2 solid walls and therefore it be part of the multiphase flow course, right and then we will have actual 2 phase 2 liquids, okay.