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

Lecture - 32 Turing patterns: Instability in reaction-diffusion systems

So welcome to today's lecture. What we will do today is talk about a stability problem again but this will be something which does not involve any fluid motion okay and in particular we are going to talk about Turing patterns. So Turing patterns are basically patterns, which arise when you have an interaction between a reaction and diffusion okay and the motivation for this is you would have seen many patterns on the animal skin.

For example, you have the zebra which has stripes, white and black stripes, you have the leopard, you have the tiger, which has a pattern and so the question is how do these patterns arise? Is there a way for you to actually describe the formation of these patterns okay? So of course there is a theory which has been proposed and that is what we are going to discuss and what we will discuss at the stage is the basic theory, which does not involve any fluid motion okay.

But the emphasis is in just understanding how reaction and diffusion and what are the kind of features reaction have to possess for you to actually see these kinds of patterns. So with whatever we have done so far in the course, we should be able to get some insight about this okay. The basic idea is when an organism is growing okay, there are many cells which are going to start with one cell, it divides, it proliferates, lots of chemical reactions going on.

There is also transport primarily by diffusion. So if the chemicals are going to be such that there is going to be reaction and there is going to be diffusion. Is it that possible that if these can rearrange themselves which can finally give rise to some kind of a pattern okay? So this is something which is not being forced by anybody outside but is just that the intrinsic feature of the system is what is causing this.

So whether this can actually give any insight into the formation of patterns, so what we are going to talk about today is Turing patterns.

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And possibly another keyword for you to search is morphogenesis okay. So what are you trying to do? We want to understand formation of spatial patterns on animal skin, for example the stripes on zebra, maybe the spots on a leopard etc, etc okay. So that is what we want to try and do. Idea is during the growth of the embryo, we have chemical reactions and cell proliferation okay.

The cells are going to multiply and they are going to grow okay and the chemical reaction also taking place simultaneously. So is it possible that the interaction between these chemical reactions and as the thing grows there is going to be some kind of a gradient in the concentrations okay. Is it possible that this gradient and the concentrations can actually give rise to some kind of a pattern formation okay? That is the question we are asking okay.

Can gradients in concentration arise in the presence of reaction and diffusion? That is the question okay. So the question which Alan Turing basically asked is this Turing patterns have been in the name of the fellow who actually started this was. Let us consider a system where there is no diffusion taking place. So to begin with we will keep the system very simple, will talk about only 2 variables, which are actually interacting with each other.

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So let us say that u and v are concentrations of 2 chemical species okay and the idea is that the reaction going on between these 2 species and the reaction kinetics is going to be defined in terms of some kind of an expression okay, first order, second order whatever it is. So we like to know if we have no diffusion okay, the concentrations of u and v change due to reaction okay.

And that is going to be given by du/dt=f of u, v and dv/dt=g of u, v. So what is f and g representing? They represent the kinetics. Clearly, the kinetics will depend upon the concentrations of species u and v and I am just writing it in a very abstract form is I am telling you this because one of the questions we are asking is what should be the property which f and g has to possess in order for you to actually see a spatial pattern?

That is the question, which we are trying to ask. It is not that if you put first order reaction here and second order reaction here it is going to happen. So there are certain properties which f and g have to possess and that is one of these properties okay and we would like see whether our analysis in terms of this linear stability that we have been doing so far can actually give us some insight.

This analysis is slightly different in the sense that we do not need to worry about things like kinematic boundary condition and stuff like that, u and v remember are concentration of species. That is the only similarity, u and v earlier were velocity components but here is concentration of species okay. So f and g represent reaction rate expressions okay. Our question is what should be the property or features of f, g to get patterns.

That is what we are asking, so what we are going to do is we are going to pose the problem as follows. We are going to find a steady state for this system okay and you all know how to find the steady state for this system.

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So the steady state is given by f of uss, vss=0, g of uss, vss=0 that is the steady state. Clearly, it is spatially uniform. There is no concentration gradient okay. So it is spatially uniform. The variable is only a dynamic system; it does not change with space. Now I am going to assume it is a stable steady state okay. Assume this is a stable steady state. Now I am going to add diffusion to the system okay.

I am going to say that earlier my steady state was spatially uniform. Now I am going to add diffusion and when added diffusion what is going to happen? I will have a spatial dependence right. Normally, our understanding of diffusion is diffusion is something which helps you to homogenize concentration. Supposing in a vessel there are 2 regions, one with high concentration, one with low concentration what will diffusion do?

As a result of diffusion, everything becomes uniform. If you wait for a sufficiently long time, if diffusion is added to the system as a mass transfer mechanism, then at the end of the day it will have concentration make uniform everywhere right. So if I want to add diffusion, you would normally think diffusion has the tendency to homogenize concentration gradients. It will not create concentration gradients okay.

So what we are going to do now is we are going to add diffusion to the system here and say that actually that is reaction and diffusion both taking place and we are going to ask the question whether diffusion can actually destabilize the system, whether adding diffusion can actually result in an instability which can give rise to a spatial pattern okay. The basic idea is the same as whatever we have done so far in our earlier examples.

But then so the methodology is going to be the same. We have a steady state, we do the linearization and then we talk about this stability okay. So what we are going to do now is we add diffusion to the system okay. Diffusion homogenizes concentration variations; it makes the concentration uniform in a system. Our question is can diffusion and reaction give rise to patterns?

And if the answer is yes what are the conditions? What are the properties which f and g have to satisfy okay? That is what we are trying to do okay?

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Let us come to the problem where we have the spatially uniform system, which is at that (()) (14:54). So we say that the steady state this is a 2-dimensional system right. If I tell you that the steady state is stable and that is the assumption which we are making, we are assuming that the steady state is stable; the spatially uniform steady state is stable. What do you infer from that?

The uss, vss is stable okay that is given to you. Now if it is stable that means if I had done the linearization and if I had calculated the Eigen values and this is what the people have done

earlier in the course then the Eigen values are going to be negative okay and this will happen when your Jacobian matrix, the matrix which comes on linearization satisfies certain properties right.

So what is the Jacobian matrix? This implies that the lambda's of the Jacobian matrix J have negative real part okay and what about the Jacobian matrix itself? It is the partial derivative of f with respect to u, partial derivative of f with respect to v, g is respect to u, g with respect to v okay. I mean if you do the linearization that is what you would get and write it in a vectorial form.

You have done this earlier in the course. Now what about the Eigen values of the system? How do you find the Eigen values?

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The determinant of J-lambda I must be=0 or the determinant of fu-lambda fv gu and gvlambda the determinant must be=0 okay.

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So this implies fu-lambda times gv-lambda=0 or lambda squared-lambda times okay. Now I am not going to prove this but you can prove this to yourself. The conditions for stability this is stable, this has a real part of lambda negative if fu+gv is negative and fu gv-fv gu is positive okay, which basically means the trace of J is negative and the determinant of J is positive.

Remember I just want to emphasize that this is true only for a 2-dimensional system what I have written here. If you have a higher order system, this is not true okay. If you have a third order system, you need additional conditions and in fact these conditions will change. The point I am trying to make here is basically if the trace is negative that means this particular polynomial will have no change in the signs of the coefficients of lambda.

This is positive, this is positive, that is positive and if you go back one of the necessary conditions for roots to have negative real part is no sign change. It is also a sufficient condition for a quadratic. For higher order systems, you need additional conditions okay. So this no sign change is a necessary and sufficient condition for quadratic, but this is just basic theory, you can you know analyze this in many different ways.

And you can come to this conclusion, so what I am trying to tell you here is that I have assumed that the spatially uniform state is stable that means my f and g satisfy these conditions, yeah. **"Professor - student conversation starts."** These are calculated at the steady state correct. This is evaluated at the steady state. Yes, the derivatives have evaluated at the steady state.

Because what I have done is I have done the linearization around the steady state okay. So these are calculated at the steady state. So now what we want to do is this is given to me okay, you are right this is at the steady state, I am talking about the steady state not in general. Now what I want to do is I want to go back and introduce my diffusion. So I introduced my diffusion, I introduce my spatial derivative. **"Professor - student conversation ends."**

It also increases the mathematical complexity so do you have a partial differential equation alright. So what I am going to do is I am going to solve look at this system.

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We have du/dt, when we add diffusion, I have du/dt=Du d squared u/dx squared+f of u, v and dv/dt=Dv d squared v/dx squared+g of u, v. What I want to emphasize here is I am taking 2 different values for my diffusion coefficient okay. Basically, I want to have some flexibility, I do not want to say that the 2 species are you know diffusing the same rate that means I am constraining myself.

I want to you know make me special pattern happen so I want to have as much flexibility as I want to have this happen to make it happen. So I am keeping du and dv different okay. The diffusion coefficients are different, to keep my life simple I am just assuming transport only in one direction, only in x direction okay, just like what we were doing earlier. If you want to complicate your life, you can do other things.

But I just want to introduce diffusion, we are doing at one direction and as always what we will do is we will look for an infinite span in the x direction because then that helps me look for periodic solutions in the x direction okay and then we can find what the critical wave number is, critical wavelength is if there is one okay. So du and dv are different okay to get flexibility and then in the x direction we have an infinite extent.

The point is even if you did not have infinite extent, if you had a finite extent and if you prevented the species from leaving the boundary okay, which means the flux is 0, du/dx is 0. So in finite extent means there is no boundary condition I am imposing, but if you had a finite chamber and if the species cannot leave that means the flux is 0 that means the derivative is 0 okay.

If we have a finite extent in the x direction and the species cannot leave then what are the boundary condition I am going to have? du/dx=dv/dx=0, derivatives are 0, no flux okay. Why am I talking about this? Because I want to emphasize that if uss, vss is a solution to this system. Then uss, vss is also a solution to this system, is also a steady state solution.

For the infinite span, it does not matter; it goes off to infinity I am not talking about boundary conditions at all. For a finite span if I had flux is 0 then constant means flux will be 0 okay. So if uss, vss is a solution, the steady state for the system without diffusion is also a steady state for the system with diffusion okay. It satisfies the differential equations and it satisfies the boundary conditions okay.

So it is a steady state. Now the question is, is it stable okay? So if it is stable that means that is the state you are going to see. If it turns out that it can be unstable now what I have done is I have introduced 2 additional parameters du and dv, so the rates of these diffusions can possibly make something, which was stable, unstable. So that is basically I want to try and get conditions for this instability and spatial patterns in terms of these diffusion coefficients and in terms of f and g, that is the idea okay.

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So uss, vss is a steady state of the reaction diffusion system where there is reaction there is diffusion because uss is constant, so second derivative is 0, time derivative is 0, f is 0 already okay. Same thing for v, it satisfies boundary conditions. Question is, is this steady state stable? And clearly the stability of the steady state will depend upon the diffusion coefficients because these are the 2 additional parameters, which have come into the picture okay.

Depending upon the diffusion coefficient, this can be stable or unstable. So what you want to do is we want to find out if at all it is possible to have conditions on du and dv the diffusion coefficients, which can make this unstable okay. So what do we do? We do a linearization of the reaction diffusion system okay. We linearize the reaction diffusion system so what we have u tilde=u-uss, v tilde=v-vss okay.

These are my perturbation variables and these are small okay and I substituted over there in that equation and how do I get? du tilde/dt=Du d squared u tilde/dx squared okay+you do the linearization of f around the steady state you get f sub u u tilde+f sub v v tilde okay and we get dv tilde/dt is this clear? So all I am doing is I mean you all are experts in doing linearization by now, I am just linearizing okay+gu u tilde+gv v tilde okay.

Now I make sure I have not done anything silly, great, yeah "**Professor - student** conversation starts." And the boundary, yeah, correct, this is at the boundary. (Refer Slide Time: 29:12)

That is my boundary condition. So what I have to do is I will do what I have done earlier, write this in a vectorial form okay and I am going to write okay. We will talk about the situation where it is infinite in extent okay. **"Professor - student conversation ends."**

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So what do I do, u tilde is a function of extent t and I am going to write this as u star e power sigma t time sin alpha x infinite to the x direction, so I am looking a periodic solution in the x direction okay. It is linear so I am talking about the linearize problem, grows exponentially in time and in Laplace transform, Fourier transform and that is the amplitude okay. We are looking for conditions under which I have nonzero u star.

So now I am going to substitute this in our equation over there and when I put du tilde/dt, I get sigma e power sigma t sin alpha x u star=Du, when I differentiate this twice I get –alpha

squared Du u star e power sigma t sin alpha x+fu u tilde is u star e power sigma t sin alpha x then+fv v star e power sigma t sin alpha x. So u and v are basically kind of in phase spatially okay. What happens now?

I can actually strike off this e power sigma t sin alpha x everywhere. That tells me that the assumed form of the solution is a possible solution okay. If I could not have done this striking off that means what I have assumed is wrong. I am assuming v tilde and u tilde both are the similar form okay. V tilde is also of the same form, same thing. So this gives me sigma u star=-alpha squared Du u star+fu u star and then+fv v star.

If you did the same thing for the other equation, I have done this for one equation, I am going to do it for the other equation. I will get sigma v star=-alpha squared Dv v star okay+gu u star+gv v star okay. That is what I would get. Now actually the sigma is my Eigen value which tells me where is stable or unstable okay. I had lambda earlier but sigma is the growth rate. The real part of sigma being negative indicates stability remember that.

So I am going to write this in a vectorial form. When I write this in a vectorial form, I get sigma u star v star=fu-alpha squared Du fv u star is gu and I had gv-alpha squared Dv okay. So what we have done is I have just added diffusion, the steady state is the same. I am doing the linearization to find out the stability of the steady state okay. When I do the linearization, I follow the usual method and take order of epsilon terms.

These perturbations are of order epsilon, so just take the first order terms okay and then I get these linearized equations. Since it is infinite in the x direction, I am looking for periodic solutions in the x exponential in time is first order and I proceed and when I proceed this is what I get and this is exactly what you people did earlier in your other stability problems okay.

Now I want you to understand that this is my Jacobian matrix, which has a diffusion included. So earlier when we did not have diffusion, these guys were 0 okay and we had a Jacobian matrix containing only these 4 elements. Now when the diffusion is included, I am getting on the diagonal elements 2 extra contributions okay and that is what is basically being reflected here.

Now since this is again a 2-dimensional system, what are the conditions for stability? The conditions for stability are that the trace must be negative and the determinant must be positive correct. I mean because it is a 2-dimensional system. What all I am saying is now the Jacobian matrix is modified okay.

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We have a modified Jacobian matrix okay and the Jacobian matrix is given by fu-alpha squared Du gu fv and gv-alpha squared Dv. For instability of the steady state with the diffusion added either trace must be negative, let us do like this, let us talk our stability state. For stability of the steady state, the trace of J must be negative okay. Trace of J must be negative means fu+gv-alpha squared times Du+Dv must be negative.

That is when diffusion is added I want the steady state to be stable, so when will that happen? I am looking at the one condition first, I am looking at this condition, now what do I already know in the absence of diffusion I have already said that the system is stable because if the system is unstable for the without diffusion then there is no point in talking about the stability with diffusion okay.

So I already know that fu+gv is negative, fu+gv is the trace of the system, so given we know or we have fu+gv is negative that is what we started off with. So if fu+gv is negative and alpha squared of course is positive, diffusion coefficients are positive that means this is always going to be negative. So what I am trying to say is that for the system with the diffusion, the trace is always going to be negative okay. So when we add diffusion, trace is always negative that means the trace condition cannot be violated and it cannot give you an instability okay. Now we have to look for the other condition because both the conditions have to be satisfied simultaneously, the trace and the determinant. In order for you to be stable in order for this 2-dimensional system to be stable, the trace and the determinant both have to be satisfied.

I am saying that the trace is satisfied, now what about determinant? Let us look at the determinant of the system. So that determinant of that system tells me, yeah **"Professor - student conversation starts."** Yes. No, no steady state is the same. See the earlier problem the diffusion was not there okay. So I had a particular steady state uss, vss. I have added diffusion but I am keeping the steady state the same.

So question is when I add a diffusion to the system, can the diffusion induce instability? That is what we are asking. So without diffusion it is stable, the trace is negative. The steady state is the same, so fu and gv are all evaluated at the same steady state. So like he was asking they are evaluated at the steady state. Now the steady state with the diffusion is also the same. So fu and gv all this is being evaluated at the steady state remember.

All these derivatives are evaluated at the steady state because my Jacobian matrix is evaluated at the steady state. So this fu and gv is at the steady state, which is the steady state of the earlier system. So that is the reason I am going to use the information from the earlier system. If this is another steady state, I cannot. **"Professor - student conversation ends."** (Refer Slide Time: 40:01)

The determinant of J this guy is fu-alpha squared Du times gv-alpha squared Dv okay-fv gu as the determinant and I am going to multiply this out and get alpha power 4 Du Dv-alpha squared times what? Du gv+Dv gu+fu gv-fv gu, that is my determinant of the system okay and remember all the fu, gv etc are at the steady state just to be making it clear one more time because I have done linearization.

I have done linearization about the steady state okay. So the partial derivatives are evaluated at the steady state. Now what do we know? So these partial derivatives are also going to be evaluated at the same steady state. What do we know? The determinant of the earlier system was positive, so this guy is positive right. Given from the earlier thing, this piece is positive okay. This guy is also positive; diffusion coefficients are positive.

This is also positive and clearly the only way the determinant can be negative is if this is positive because this is associated with the –sign then if this dominates these 2 terms see look at this; this is positive, this guy is positive, there is a – sign associated here. If Du gv+Dv gu is negative, if this is negative, something is wrong "**Professor - student conversation starts.**" This one, Dv fu, thank you, thank you. "**Professor - student conversation ends.**"

So if this guy is negative then everything is positive because there is a - sign here that means the determinant is going to be positive, the determinant of the system with the diffusion okay that means then the determinant of the R-D system is positive and my steady state is stable okay. If at all you want to have instability of the spatially uniform solution, then this has to be negative okay.

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So for instability Du gv Dv fu must be positive and is it a necessary condition or a sufficient condition? It is a necessary condition just because it is positive we are not assured, it will be negative, it has to be significantly large only then. So this is necessary condition just because this is positive it will not guarantee you that you will have instability okay. This is a necessary condition; it does not guarantee instability okay.

So now you already know something about f and g. What do we know? Some trace condition. What do we know? We know fu+gv is negative that is given to me right. So now I want to see, while looking at this condition and looking at this condition when can this happen? When can I possibly have instability? When can I possibly have spatial pattern? Okay. If this is negative I have 2 options both are negative individually or one is positive, one is negative okay.

If both of these are negative then I cannot satisfy this, agreed okay. If this fu is negative, gv is negative then this is always be a negative. If therefore one has to be positive and one has to be negative, then one is positive one is negative and then maybe I can satisfy this condition you understand. So both fu and gv cannot be negative since then Du gv+Dv fu will be negative always okay.

So now I got a choice you can choose whatever you want. I am going to choose fu to be positive and gv to be negative okay. So let us choose fu to be positive and gv to be negative, it does not matter, it can be chosen in the other way, it really does not matter okay. So I am

choosing fu to be positive and gv to be negative and if that is the case what exactly does this imply? Remember f occurs in the mass balance equation for u du/dt is f of u, v okay.

And dv/dt is g of u, v right. If the partial derivative of f with respect to u is positive that means as the concentration of u increases, the reaction rate is increasing okay and that is typically what you expect. If you have a first order reaction or a second order reaction, you say that the more the concentration the more the reaction rate.

So this is a normal behavior whereas for g for here gv is negative that means as a concentration of v is increasing, the reaction rate is actually decreasing okay. So here this is as the v as it increases it actually slowing down the reaction. So in some sense you can think of this species u as an activator that is the more the u, the more the reaction rate. v is an inhibitor the more the v, the lower is the reaction rate okay.

So this is something which we have understood now that in order for you to possibly have instability, you need to have an activator and an inhibitor okay. Now we have to do this analysis some more but we will do that in the next class, but all I wanted to emphasize here is u is an activator. Why? Because as the concentration of u increases the reaction rate increases.

V is an inhibitor. Why? Because as the concentration of the v increases, the reaction rate decreases. So basically you need to have a combination of an activator and an inhibitor in your reaction system in order for you to actually have pattern if at all. Of course this is just a qualitative argument. What we need to do is get conditions on a diffusion coefficient okay.