Advanced Mathematical Techniques in Chemical Engineering
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Lecture No. # 06
Contraction Mapping

Good afternoon everyone; we will be continuing our discussion on contraction mapping. Contraction mapping is one of the important chemical engineering mathematical techniques and that can be used quite widely for determining the steady state of a typical chemical engineering process. In the last lecture, we have seen, what is the theory behind contraction mapping and how a sequence can be giving a converged.

How a sequence, under what conditions the sequence can be boiled down to a convergence sequence? A function will be converging to a particular point in the domain and that particular point is called the steady state or the fixed point of the system. The steady state is very important and we are basically going to study what are the conditions of the system that will lead to a unique steady state.

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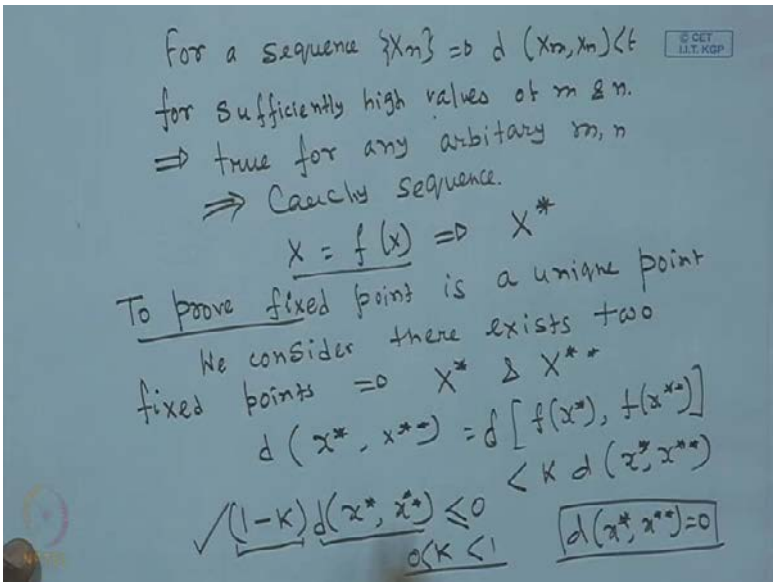

Now, we have learnt in the earlier class that for a sequence X n it will be the metric between X m and X n is less than epsilon for sufficiently high value of m and n. Since, it is true for any arbitrary m and m. This sequence is a Cauchy sequence but therefore, the map X is equal to f x it will converge to a fixed point called X star.

We have to prove that this fixed point is a unique fixed point that means, we have to prove the obtain steady state is the unique steady state. To obtain that we do the logic of negative reasoning, so we consider there exists two fixed points: these are X star and X double star. Therefore, if we calculate the metric between these two fixed points: d metric between X star and X double star should be nothing but metric between - this relationship has to obey for the both the cases - metric between f x star and f x double star. Since, we have proved that f is a contraction map, this should be less than k d metric between x star and x double star.

Now, we can change over these and we can bring this thing on the left hand side. The metric between x star and x double star being a scalar it can be taken out and can be taken it has common. So, the equation becomes metric between x star and x double star multiplied by 1 minus k should be less than equal to 0.

This is ever positive, the k is a fraction lying between 0 and 1, 1 minus k is always positive then, in order to satisfy this equation and this metric which is ever positive. So, multiplication of the two positive quantities cannot be negative. So, the only option that is left is the metric between d x and x double star should be equal to 0 in order to satisfy this equation (Refer Slide Time: 04:38).

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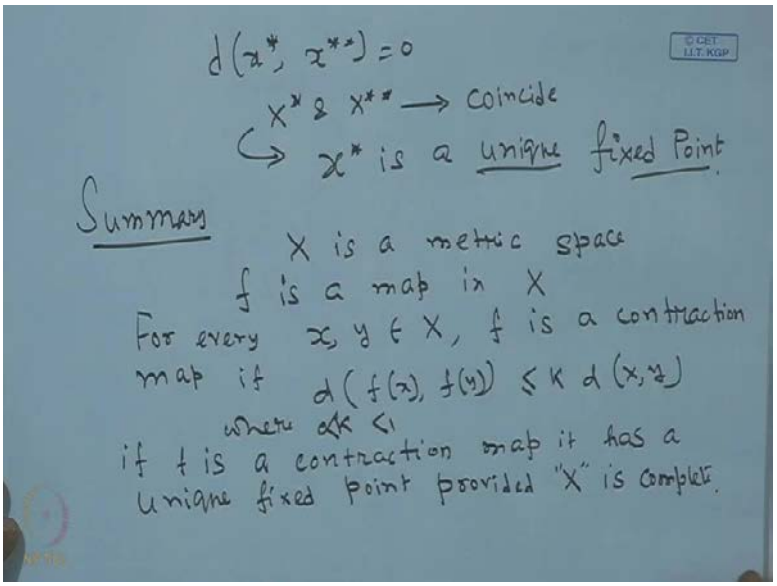

Therefore, the metric between x star and x double star turns out to be 0 that simply means we are talking about the same point, so x star and x double star they coincide.

Since they coincide, we are talking about that x star is a unique fixed point. We are talking about the condition of unique fixed point. So, let us summarize whatever we have done till now.

We considered x is a metric space and f is a map in space x then, for every value of x and y belonging to space x, f is defined a contraction map if metric between f of x and f of y is less than equal to k times metric between x and y, where k is a fraction lying between 0 and 1. Now, if f is a contraction map, it has a unique fixed point provided space x is complete. So that goes the mathematical definition of fixed point and the unique fixed point or the contraction map.

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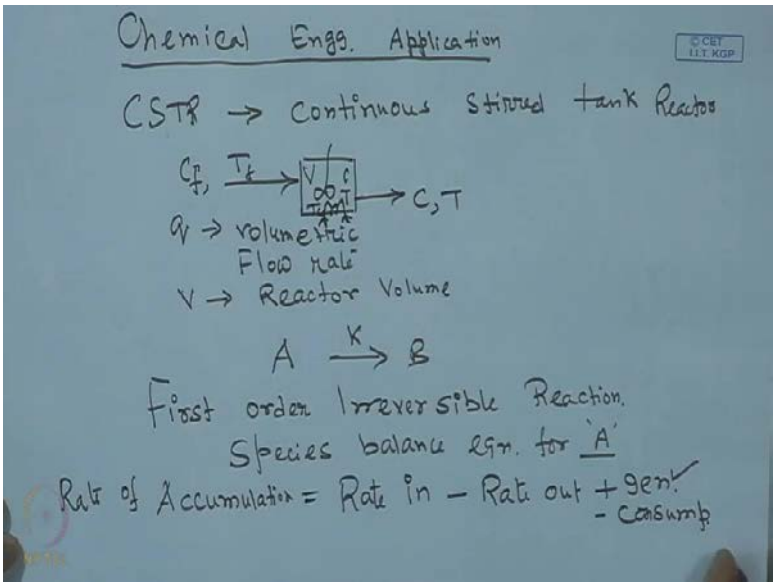

Let us look into one of the chemical engineering applications. Typical chemical engineering application occurs in the field of reaction engineering. In this field, what we can do? By adopting the contraction mapping method, one can identify the set of the operating conditions for which one can get the unique fixed point or unique steady state condition.

We talk about a reactor it is known as CSTR. CSTR is known as Continuous Stirred Tank Reactor. This reactor is known to all chemical engineers and it is to consider a non-isothermal CSTR; it is a stirred cell, where the materials are going into at a concentration C f and temperature T f. Within the reactor it is well stirred therefore, it is assumed the reaction volume or reaction material inside the reactor is well stirred; it is uniformly

stirred everywhere and the concentration that is prevailing inside the reactor is C and temperature T. The same concentration we are going to get at the output at the stream that we are drawing out. So, q is the volumetric flow rate, v is reactor volume and there is a jacket has been placed, where we are putting the coolant liquid at temperature T c.

Now, we are considering a first ordered irreversible reaction is going on inside the reactor A going to B with a rate constant k; this is first order irreversible reaction. What we will be doing? We will be doing a species balance for this particular set of reactant A. We write down the species balance equation for A and any balance equation is in the form of rate of accumulation is equal to total rate of material that is going into the system minus rate of material that is going out of the system plus rate of generation minus rate of consumption.

Now, if we are writing down a balance equation for the reactant A then, there is no rate of generation that is having in the system. The reactant will be consumed and the rate constant is given by the rate expression.

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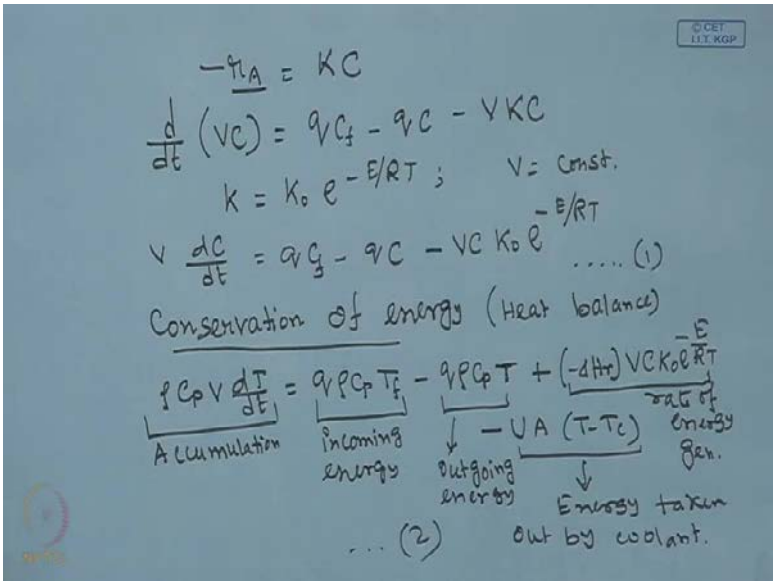

The first order kinetic rate expression and the rate expression is given as minus r A is equal to K times C. We write down the balance equation for the reactant, so d d t of V times C is equal to material that is going into the system is q times C f minus q times C that is going out minus rate of consumption will be V times rate expression; V times

minus r A. So, V into K into C that is the how the rate of the reactant that is consumed into the system as a reactant.

The rate constant K is written as in terms of Arrhenius constant coefficient as K naught into e to the power minus E by RT. So that gives a complete expression and in our whole analysis the reactor volume is kept as constant. We can write v times d c d t is equal to q times C f minus q times C minus VC K naught e to the power minus RT. So, this equation is the mass balance equation, it is indeed a solute balanced equation, it gives the total balance of the reactant.

Next equation that we are going to write is the conservation of energy or heat balance equation. Again, we will be writing the same thing, like rate of accumulation of energy is equal to rate of energy that is going into the system minus rate of energy that is going out of the system plus rate of energy, which is an exothermal reaction. So, amount of energy that is getting out of it and the material that is taken out to the coolant, so rate of energy taking out.

If you write down the conservation of energy, the first term will be rho C p V times d T d t; this gives rate of accumulation of energy minus q rho C p T f is the energy by which the energy getting into the system. The incoming stream q rho C p T is the rate by which the energy is flowing out of the system plus minus delta H r V time's C k 0 e to the power minus E by RT that is the exothermic. The rate of energy that is developed into the system, because of the exothermic reaction minus U times A T minus T c energy going out of the system.

So, this is the accumulation term; rate of accumulation, this is the incoming energy, this is out going energy, this is rate of energy generation and this is the term the rate of energy taken out by the coolant (Refer Slide Time: 14:32). We write down the mass balance equation, species balance equation and the energy balance equation; this is the second equation. We will working on these two set of equations, but before that we should make the parameters dimensionless, so the variables becomes well behaved within the range of 0 to 1.

Let us do the non-dimensionalization of the parameters.

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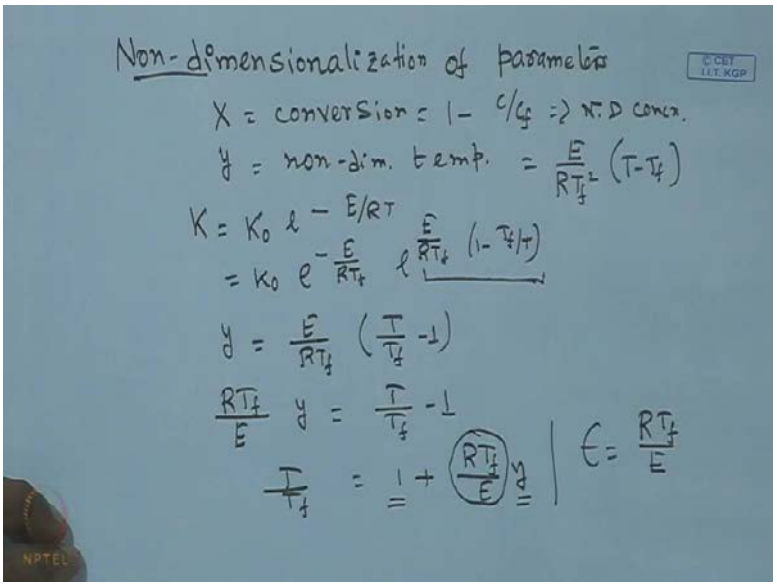

The first non-dimensionalization parameter is the non-dimensional concentration, where is given as conversion. The conversion is given as 1 minus C by C f; C is the concentration at any point of time divided by C f is the fit concentration 1 minus that is nothing but the conversion.

We defined y as non-dimensional - so conversion is non-dimensional concentration - y is non-dimensional temperature this is defined as E over RT f square T minus T f. We defined k as the Arrhenius rate law e to the power minus E over RT. This becomes k 0 e to the power E by RT f, you add and subtract, so it becomes e to the power E by RT f 1 minus T f by T.

Let us work on this equation, so y is we take 1 T f inside E by RT f we take 1 T f inside, so this becomes T minus T by T f minus 1. So, RT f by E times y will be nothing but T by T f minus 1. So, T by T f can be written as 1 plus RT f by E multiplied by y (Refer Slide Time: 17:25). In this equation the left hand side is completely non dimensional and the right hand side there are two terms: one is completely non dimensional, in this term y is non-dimensional that means RT f by E has to be a non-dimensional number, we call that as epsilon; write epsilon is equal to RT f by E, E is the activation energy.

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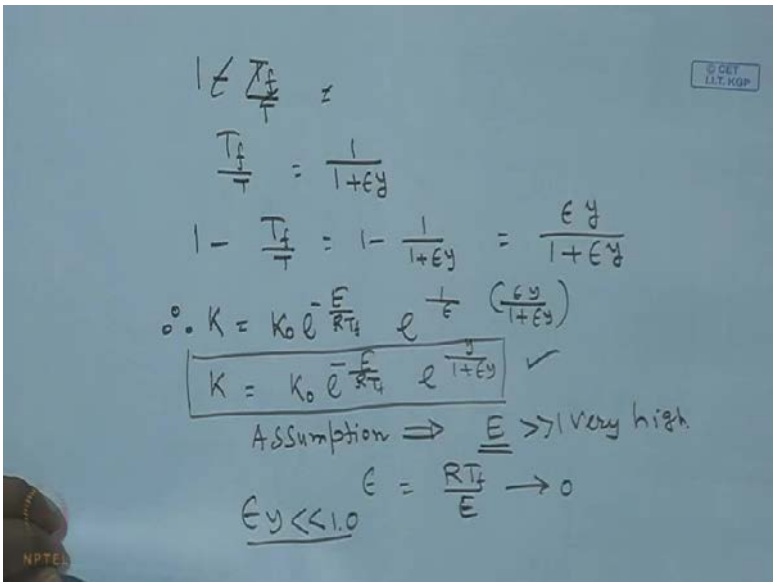

We write as 1 minus T f by T is equal to - so T f by T is how much? So, T f by T is nothing but 1 over 1 plus epsilon y. If that is the case, then 1 minus T f by T give you 1 minus 1 over 1 plus epsilon y. So, this becomes after simplification epsilon y divided by 1 plus epsilon y. Therefore, we can express K as K 0 e to the power minus E by RT f into e to the power 1 by epsilon, epsilon y divided by 1 plus epsilon y. Finally, this becomes K 0 e to the power minus E by RT f e to the power y divided by 1 plus epsilon y.

That is how the Arrhenius rate constant is made non dimensional. We write down one assumption here; the assumption is to simplify our mathematical treatment, we have this assumption; the assumption is E is extremely high. For extremely high epsilon for activation energy E the epsilon will be extremely small RT f by E will be tending to 0. So, in that case, for high activation energy epsilon y will be much less than 1.

Under this condition this expression will be simply reduced to a much simpler amenable form and what we can do? We can neglect 1 plus epsilon y and we can neglect epsilon y terms with respect to 1 and this will be simply e to the power y (Refer Slide Time: 20:36).

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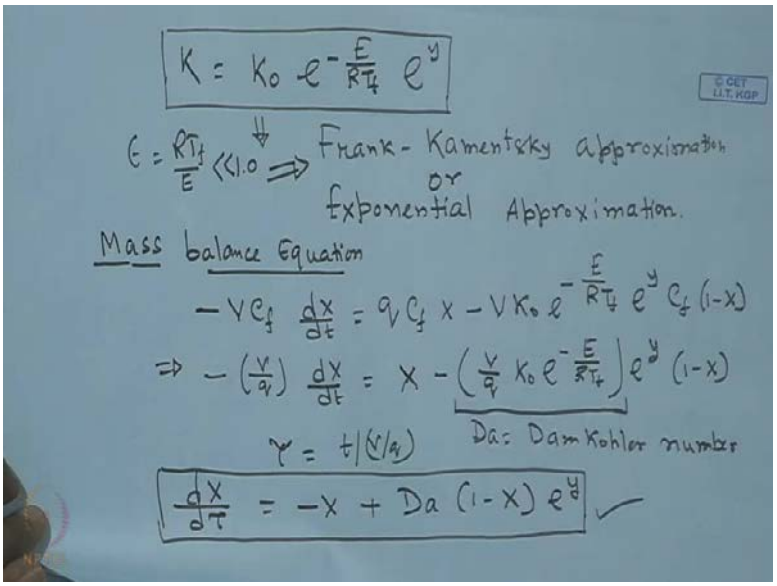

The expression of Arrhenius rate constant can be written as K is equal to K 0 e to the power minus RT f multiplied by e to the power y. This assumption is known as the Frank-Kamentsky assumption or approximation or often that is high that epsilon is equal to RT f by E is extremely small. This is known as the Frank-Kamentsky approximation or since, it is appearing in the exponential term sometimes it is also known as the exponential approximation.

Under the approximation of Frank-Kamentsky method then, we can reduce our mass balance equation and energy balance equation to more amenable form. Just look into the mass balance equation, whatever we have written in the earlier case, we make it non dimensional minus V times C f dx dt is equal to q times C f times x minus V K naught e to the power minus E by RT f e to the power y C f multiplied by 1 minus x. We make the whole thing to be non-dimensional divide both sides by C f and q. So, this will be minus v by q dx dt is equal to x minus v by q K naught e to the power of minus E by RT f e to the power y 1 minus x. Now, this whole term is non-dimensional and this is known as Damkohler number.

Damkohler number is a parameter and on the right hand side x is non-dimensional, this is non-dimensional, y is non-dimensional, x is non-dimensional therefore, on the left hand side also has to be non-dimensional (Refer Slide Time: 23:44).

Out of these there are two components; the left hand side is a multiplication of the two terms, the right hand side the t is in second. If you look into the unit of v by q v is in meter cube and q is the volumetric flow rate meter cube per second therefore, v by q is having the unit of time. Therefore, we define non dimensional time as t by v by q. This equation can be written in absolutely non-dimensional term as dx d tou is equal to minus x plus Damkohler number 1 minus x e to the power y. So, this gives the dimensionless form of mass balance equation.

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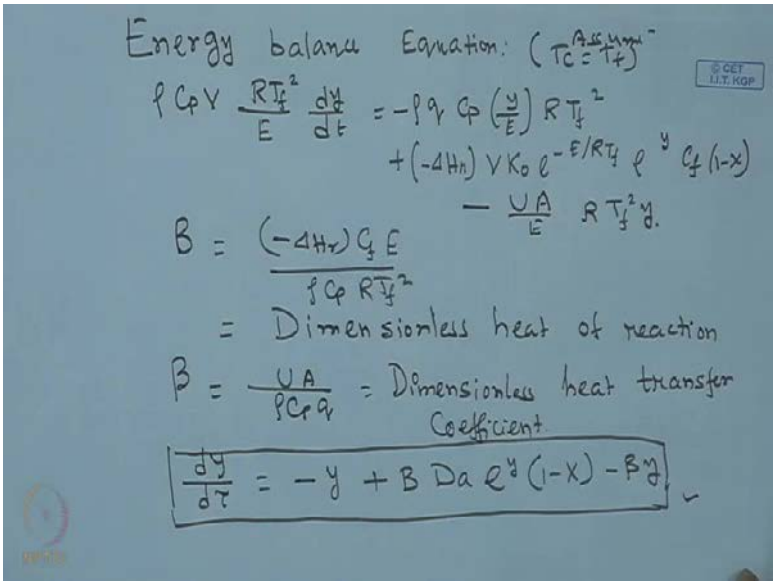

Next we do the same treatment for the energy balance equation. In this case, we make it non dimensional rho C p V RT f square divided by E dy dt is equal to minus rho q C p y by E RT f square plus minus delta H r; this is the exothermic reaction term. V K naught e to the power minus E over RT f e to the power y C f 1 minus x minus U A over E RT f square times y.

Only one assumption has been made; it has been made that T c is equal to T f. We have this assumption to have a mathematical simplification in your analysis without any loss of generality of the problem. We are assuming that the coolant temperature is getting into the system at the fit temperature that is a reasonable one.

Again, we define some of the non-dimensional parameter B is minus delta H r C f times E divided by rho C p RT f square; this is known as the dimensionless heat of reaction. We have another non-dimensional parameter beta that is U A rho C p times q and again,

this is dimensionless heat transfer coefficient. The non-dimensional form of the energy equation will be able to write it down now, dy d tau minus y plus b times Damkohler number e times e to the power y 1 minus x minus beta times y. This is the form of a heat balance equation or energy balance equation in its non-dimensional version (Refer Slide Time: 27:22). We have already seen and derived the non-dimensional version of mass balance in the couple of minutes ago.

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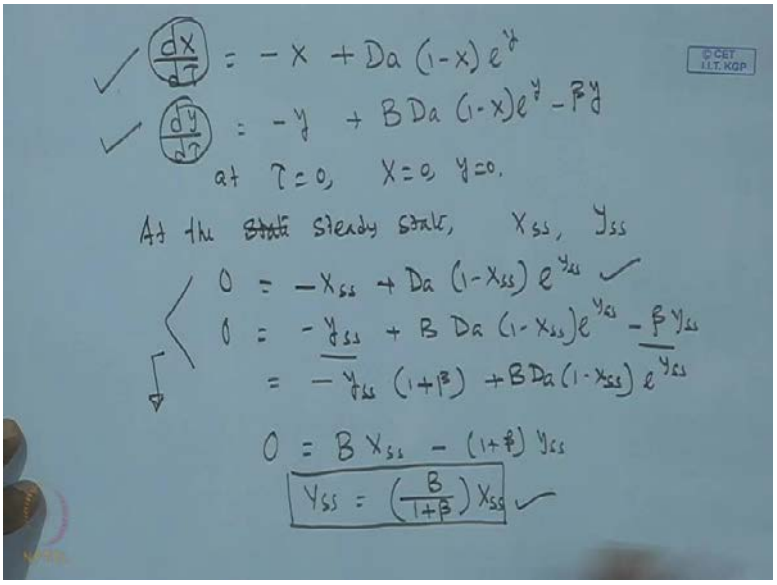

Let us just write these two equations in the non-dimensional form. The mass balance equation takes this form dx by d tau is equal to minus x plus Da 1 minus x e to the power y and dy d tau is equal to minus y plus B times Da 1 minus x e to the power y minus beta y. This two equations are solved and they are subjected to the initial condition at tau is equal to 0, x is equal to 0 and y is equal to 0.

This is the transient mass balance equation, transient energy balance equation. So, this is the equations governing for the concentration, this is the equation which is governing the temperature of the system. Now, we are not interested into the transient analysis, what we are interested in that? We are interested in the steady state process (Refer Slide Time: 28:28).

At the steady state, the state variables becomes x ss and y ss. Under these conditions at the steady state, the transient terms dx d tau and dy d tau they does not exist, they vanish. Therefore, at the steady state, we write down the governing equation minus x ss plus Da

1 minus x ss e to the power y ss. The energy balance equation will be giving you y ss plus B Da 1 minus x ss e to the power y ss minus beta y ss. We can just write them in a more amenable form, we can write it as minus y ss combine these two terms into 1 plus beta plus B Da 1 minus x ss e to the power y ss (Refer Slide Time: 29:54).

We can combine these two equation and write it down as; if we combine this two equation or we will be getting the resultant equation will be in very simple form B x ss minus 1 plus beta y ss. So, y ss will be nothing but b divided by 1 plus beta times x ss. Simplification of non dimensional form of energy balance and non-dimensional form of mass balance gives a very straight forward linear relationship between the non-dimensional temperature and non-dimensional concentration on conversion through the parameters B and beta and it is a linear parameter (Refer Slide Time: 30:05).

Now, what we can do? We can substitute y in one of these equation in favor of x and express everything in terms of x, let us do that.

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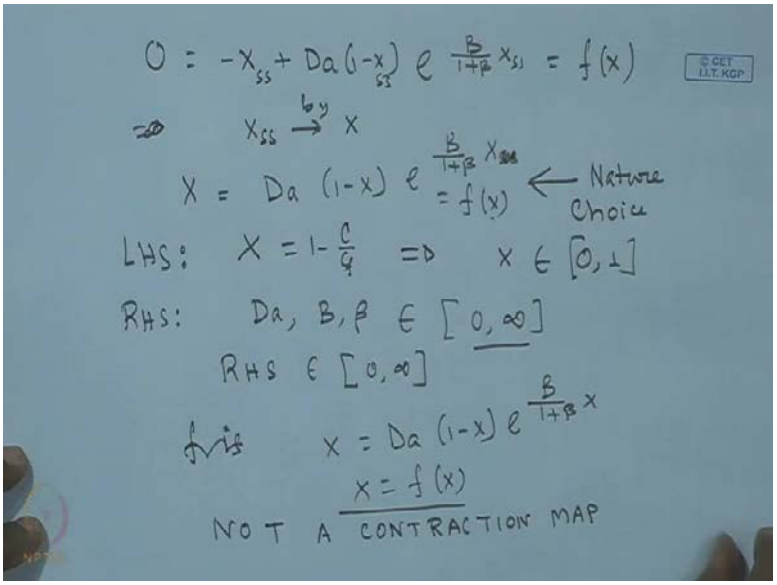

If we do that we will be getting 0 is equal to minus x plus Da 1 minus x e to the power B divided by 1 plus beta times x. We can write it in this form, so this is in steady state, now we can do with the steady state, we substitute x steady state by x. So, if you do that and take this thing on the other side, we will be getting the equation X is equal to Da into 1 minus x e to the power B by 1 plus beta times x ss.

Now, there are two ways these equation can be x ss will be written as x. This is some function of x. So, there are two ways this function can be written. The natural choice of writing this equation is this, the way it is written. Natural choice it is written as x to be taken on the other side, Da into 1 minus x e to the power B by 1 plus beta times x.

Now, let us try to analyze this expression. In this expression, if you see the left hand side, what is left hand side? It is nothing but conversion C by C f. C by C f is always a fraction therefore, 1 minus C by C f a fraction, as a result x is always a fraction in the domain of x is from 0 to 1.

On the other hand, this is the status of left hand side, the status on the right hand side is that in this case, Da can be assuming any value up to - I know it is Da B and beta these parameters they belong to the domain 0 to infinity. If that is the case, the right hand side can be also belonging to 0 to infinity. Therefore, the domain of left hand side and the right hand side does not match.

If we take up a value, so if we write x is equal to - let say, this is x is equal to f x then, the x belonging to the domain 0 to 1, where f is a map it takes up a value in the x domain operates on it but, it retains the value in the 0 to infinity domain. The way we have written x is equal to f x from this equation is not proper. So, f is not a contraction map in this case.

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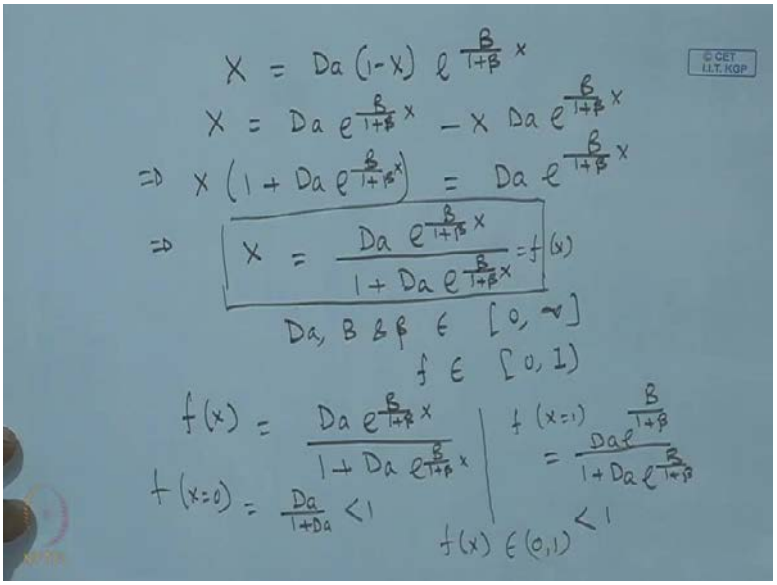

If we write x is equal to Da 1 minus x e to the power B by 1 plus beta times x is equal to f of x; this is not a contraction map, because the domain of left hand side does not match with the domain on the right hand side. We have to rewrite this equation from the starting point once again. We write it x is equal to Da into 1 minus x e to the power B divided by 1 plus beta times x. We just multiply this equation by this exponential term. So, this is Da e to the power B by 1 plus beta times x minus x times Da e to the power B by 1 plus beta times x.

We take x to the left hand side, so this becomes 1 plus Da e to the power B plus 1 by beta times x is equal to Da e to the power B by 1 plus beta times x. Divide this by this equation, so we will be getting x is equal to Da e to the power B by 1 plus beta times x divided by 1 plus Da e to the power B by 1 plus beta times x. So, this we write down as f of x (Refer Slide Time: 35:12).

If we recast the f of x in this form, we can see that for any value of Da B and beta lying in the domain 0 to infinity, this will be effects the right hand side will be always a fraction. This something divided by 1 plus something, so it will be always a fraction. So, f is belonging to the domain 0 to 1 always.

For example, if we plot, so what is f x then? The f is Da e to the power B by 1 plus beta times x divided by 1 plus Da e to the power B by 1 plus beta times x. For x is equal to 0 this becomes Da divided by 1 plus Da so, this is less than 1. If we put the maximum value of x f x is equal to 1 this will be Da e to the power B divided by 1 plus beta divided by 1 plus Da e to the power B divided by 1 plus beta, so this is also less than 1.

So, f x for whole domain of x lying between 0 and 1; f x is also lying between 0 and 1. Really, we are now mapping the What f is doing now? The f is taking up a value from the x domain, which is between 0 to 1 and it is mapping on the same domain in 0 to 1. So, the choice of this function x is equal to f x is appropriate and we can go ahead with this.

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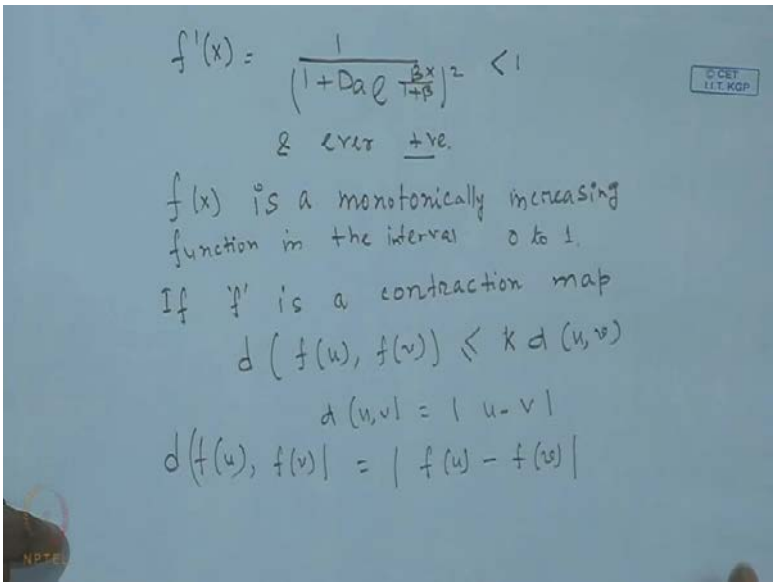

Now, if you look into the f prime x, you will find out that f prime x turns out to be 1 plus Da e to the power B x divided by 1 plus beta whole square. For the full domain of f prime x is less than 1 and it is ever positive. So, f x this simply means f prime x ever positive means, f x is a monotonically increasing function in the interval 0 to 1.

Now, f can be a contraction map; if f is a contraction map then, we have to get this equation to be satisfied, metric between f of u and f of v should be less than equal k d times metric between u and v, where metric between u and v is nothing but the distance between u and v, so it is mod of u minus v.

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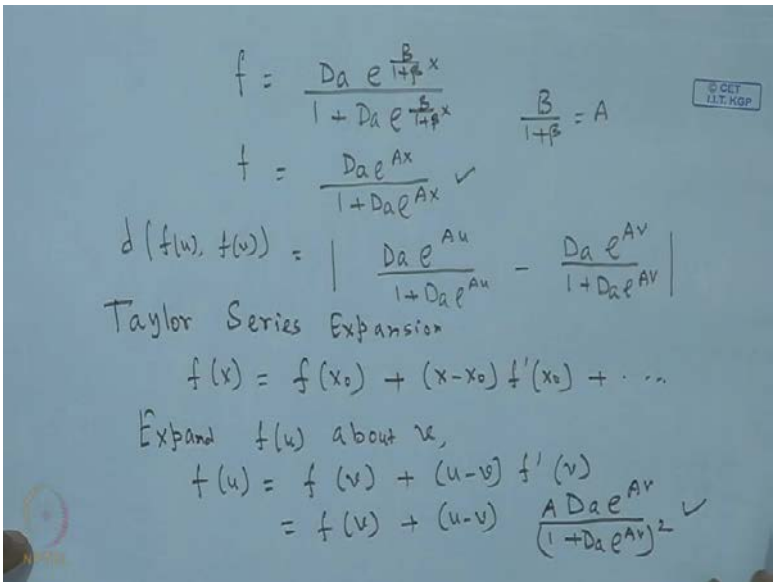

Therefore, we can write d of metric between f of u and f of v can be written as mod f of u minus f of v. We can write down the expression of f in this fashion, so if we remember what is f? The f is Da e to the power B by 1 plus beta x divided by 1 plus Da e to the power B by 1 plus beta times x. We substitute B by 1 plus beta as a parameter A, so f becomes Da e to the power Ax divided by 1 plus Da e to the power Ax. So, d of metric between f of u and f of v now becomes mod of Da e to the power A u divided by 1 plus Da e to the power Au minus Da e to the power Av divided by 1 plus Da e to the power Av mod of that.

Now, we can have a Taylor series expansion, so we can re-brush all your knowledge that what is a Taylor series expansion? The f of x can be expanded about a value x naught as f of x naught is equal to f x equal to f x naught plus x minus x naught f prime x naught plus higher order term x minus x naught square d square f x d x square evaluated at x naught.

We neglect the higher order terms, so we expand f of u about v by Taylor series expansion. The expression becomes f of u is equal to f of v plus u minus v f prime v. This is the Taylor series expansion of whatever we have done earlier. So, we just write f of v plus u minus v and what is f prime v, that is the df dx evaluated at v and that expression becomes A Da e to the power Av divided by 1 plus Da e to the power Av square of that.

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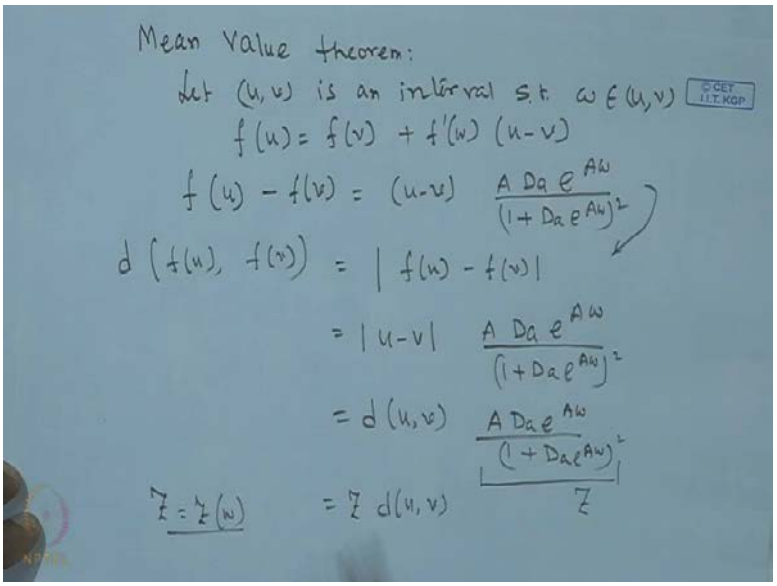

The expansion of f of u with respect to about v by Taylor series expansion is given by this expression then, we have the mean value theorem. If you remember what is the mean value theorem from our undergraduate level. The theorem said that if u and v; let, u v is an interval such that w is belonging to u and v then, f of u is equal to f of v plus f prime w multiplied by u minus v. We just substitute that so f of u minus f of v is equal to u minus v A Da e to the power Aw divided by 1 plus Da e to the power Aw square of that.

That is the case, so we are in a position now to write the metric between f of u and f of v more concrete fashion. So that will be mod of f of u minus f of v. We just write down this expression from here, so it will be mod of u minus v A Da e to the power Aw divided by 1 plus Da e to the power Aw square of that. Mod u minus v is nothing but metric between u and v multiplied by this factor A Da e to the power Aw divided by 1 plus Da e to the power Aw square. We write it as a quantity Z, so this becomes Z times metric u and v, where Z is a function of continuous variable w lying in the domain 0 to 1.

Now, this is a contraction map if and only if, the Z maximum values since, Z is a continuous function of w the maximum value of Z. So, the idea is that if this f is a contraction map metric between f of u and f of v should be less than k into d of metric between u and v that means, maximum value of Z should be less than 1. If the maximum value is less of Z is less than 1, then all the values will be less than 1.

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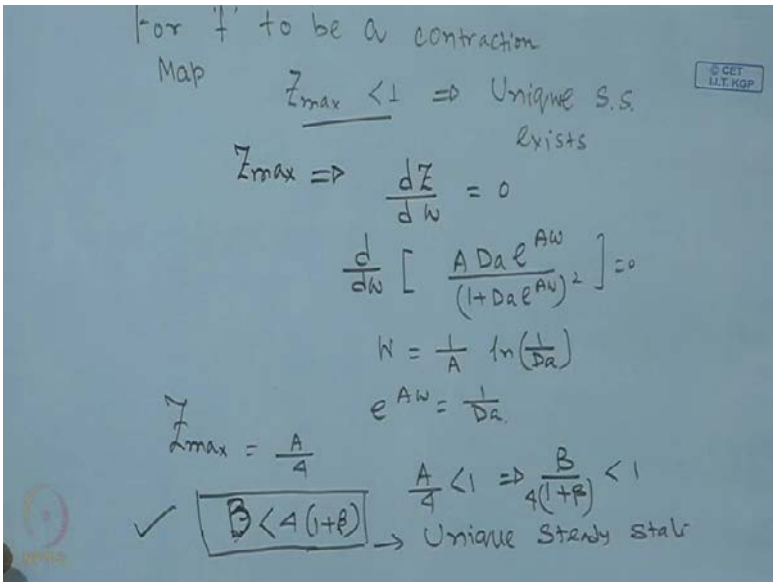

If that is the case, so we write down the condition for the contraction map. For f to be a contraction map, the Z max should be less than 1 and if Z max is less than 1 there exists a unique steady state; unique steady state exists.

Now, let us find out how Z max need to be calculated? Z max will be calculated if we write d Z d w is equal to 0. If we write d Z d w is equal to 0 that means Z is equal to A Da e to the power Aw divided by 1 plus Da e to the power Aw square of that should be equal to 0. If you solve this equation you will be finding out that the maximum value occurs at w is equal to 1 over A ln 1 over Da.

If you put back this equation here, so you will be getting e to the power Aw is nothing but 1 by Da. So, e to the power Aw is nothing but 1 by Da, substitute back into the governing equation, so Z max becomes A by 4. So, 1 plus 1 2 square, so it will be A by 4. The condition of the contraction map is Z max is less than 1 that means A by 4 should be less than 1 (Refer Slide Time: 46:52).

Let us substitute the value of A; A is nothing but B divided by 1 plus beta less than 1 4 into that. So, B is less than 4 into 1 plus beta is the condition. So, B is less than 4 into 1 plus beta is the condition for occurring unique steady state into the system. Contraction map is successfully applied for this particular system and among that there are three parameters we are having B, beta and Damkohler number. Let the Damkohler number be anything, so if the condition between B and beta; this is the relationship between the

parameters B and beta, such that B is less than 4 into 1 plus beta then, we will be having a unique steady state into this particular problem.

This example clearly demonstrates that how contractions map can be utilized to a practical chemical engineering system that is a continuous stirred torque reactor, for which we will be having non isothermal stirred torque reactor, which is very high realistic in nature. B should be less than 4 into 1 plus beta for which the unique steady state will be existing for this system.

Next, I will take up a couple of examples to illustrate this use of contraction mapping further in chemical engineering application.

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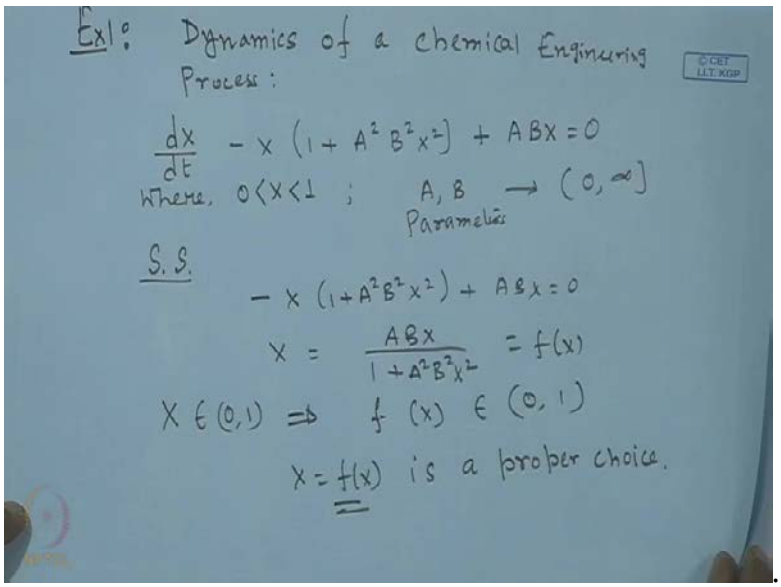

First example, I will be taking up is this 1: let us say, dynamics of a chemical engineering process is given by this mathematical expression dx dt minus x into 1 plus A square B square x square plus A B x is equal to 0, where the x lying between 0 to 1. The parameters of the system; A B are the parameters they belongs to the domain 0 to infinity, they can be assuming any values from 0 to infinity.

Now, we examine the steady state of the system and come out with a condition on the parameters, which are basically a combination of the operating conditions, for which we will be having a unique steady state to this system.

Let us first evaluate the steady state. The steady state will be evaluated from this equation when the dx dt will be equal to 0. That is the case, we at the steady state, we put dx dt equal to 0 and you will be getting this one minus x into 1 plus A square B square x square plus A B x equal to 0. So, x can be written as in this form A B x divided by 1 plus A square B square x square.

We just examine, what is the range of left hand side and right hand side? The left hand side x belongs to the domain 0 to 1 and the right hand side, we can find out that these for any value of x between 0 to 1, the function will be having let us say, for x equal to 1 maximum value of x is will be assuming as 1. So, for that A B divided by 1 plus A square B square so it will be less than 1. So, write for any value of x lying in the domain 0 to 1 f of x is also lying in the domain 0 to 1. The map x is equal to f x is a proper choice and there is a potential chance that this map can be treated as a contraction map and we can identify the conditions those will be coming out or if this map is a contraction map.

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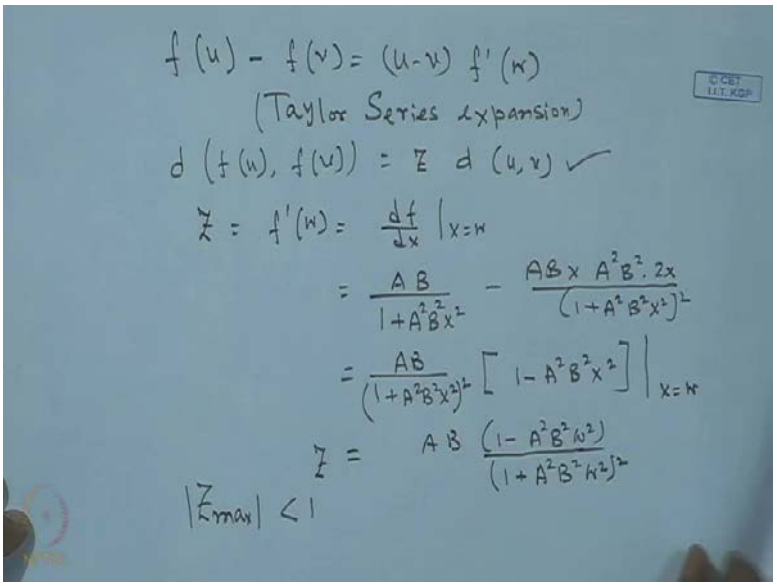

If that map is a contraction map then, we use the formula f u minus f of v is equal to u minus v multiplied by f prime at w, but w lying between u and v and this relationship we get from the Taylor series expansion. We make this analysis further, metric between f of u and f of v becomes Z times metric between u and v. If you remember what is Z, Z is nothing but f prime evaluated at w, so it will be df dx evaluated at x is equal to w.

If you differentiate this expression this becomes A B divided by 1 plus A square B square x square minus B x into A square B square multiplied by 2 x divided by 1 plus A square B square x square, square of that. You can take this as common and the whole thing becomes 1 minus A square B square x square and the expression on the right hand side will be evaluated at x is equal to w. You will be having A B into 1 minus A square B square w square divided by - so there will be square here - so there is a lcm 1 plus A square B square w square that is the value of Z (Refer Slide Time: 54:04).

So, Z is a function of w and if this expression, the function f to be a contraction map then Z maximum should be less than 1 that is the criteria. We differentiate it once again and evaluate the Z maximum and put it equal to minus 1 and see what you get.

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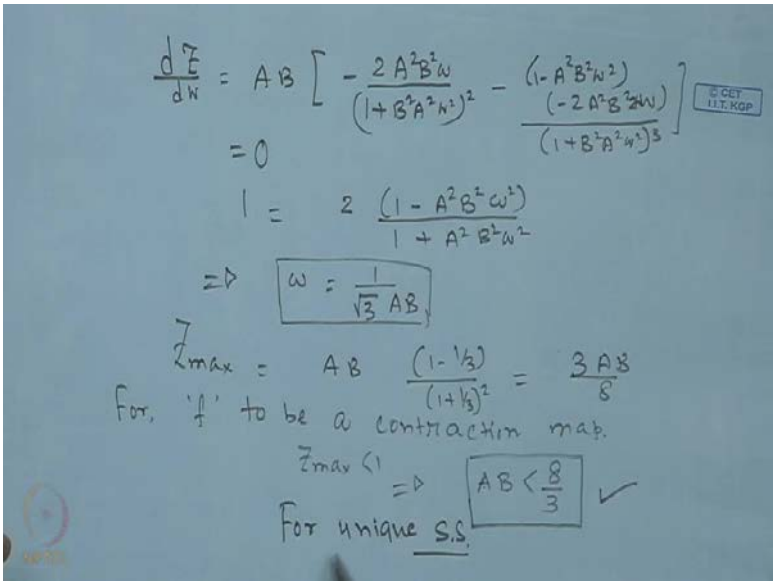

So, d Z - if you really do that you will be getting d Z d w is equal to something like this, A B minus 2 A square B square w divided by 1 plus B square A square w square; square of that minus 1 minus A square B square w square multiplied by minus 2 A square B square 2 w divided by 1 plus B square A square w square cube and put it equal to 0 to evaluate the maximum value of Z, if you do that we will be getting 1 is equal to 2 into 1 minus A square B square w square divided by 1 plus A square B square w square. If you simplify this, you will be getting w is equal to 1 by root over 3 A B.

Now, at this w the Z is maximum, so we can evaluate the Z maximum as by putting A square B square w square as 1 over root 3. So, Z maximum becomes A B into 1 minus 1 upon 3 divided by 1 plus 1 upon 3 square of that so you will be getting 3 A B by 8.

Now, for contraction f to be a contraction map, the condition is Z max should be less than 1 and we will be having A B should be less than 8 over 3. So that is the condition for which we will be having. So, this is the relationship between the two parameters A and B that is A B should be less than 8 by 3 should be there for existence of unique steady state. We will select A and B such that this is less than 8 by 3, so that a unique steady state will be existing in the system.

Similarly, we can go through some more examples, where in chemical engineering systems were the contraction mapping can be utilized can be applied, in order to find out the combination of the operating variables or the system parameters such that unique steady state will be obtain in such chemical engineering systems. In the next class, we will be taking up some more examples to illustrate the use of contraction mapping in chemical engineering. Thank you very much.