

Advanced Mathematical Techniques in Chemical Engineering

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Module No. # 01

Lecture No. # 07

Contraction Mapping

Good morning every one. As we have discussed in the last class, we are looking into the application of contraction mapping in chemical engineering processes. We have seen that contraction mapping is a very useful tool to obtain the uniqueness of a steady state that is occurring into the system. Probably in the last class, I discussed about the importance of the steady state that is in chemical engineering. So, I would like to reiterate once again that in any chemical engineering system, the output is the most important product and the product quality is extremely important, because it has a fixed and it has a tremendous market value.

If we will be able to produce the output product to the required quality then, we will be able to market it appropriately, if it does not carryover the required quality or the properties, then the whole batch will be waste. So, there will be tremendous loss in running the whole experiment, because most of the chemical engineering system are producing materials of high volumes.

Therefore, you need to have a steady state around which the product will be produced to a desirable quality and that steady state must be a unique steady state otherwise, for the same set of operating condition, if we have multiple steady states then you may be landing up with a different steady state. So that what the product quality may be different beyond the bracket of the desirable quality parameters.

Therefore, it is very important to run the process in a restricted steady state, that steady state has to be unique steady state, but in order to have a unique steady state you must be having a good control over the operating parameters. There exists a definite relationship of the operating conditions, but the steady state will be a unique steady state.

Contraction mapping is a tool to identify the relationship between the operating parameters in most of the cases, they are appearing as non-dimensional parameters whenever you will be writing a mathematical model to describe the system.

Now, this combination of these parameters, there will be definite relationship between these parameters, which will be dictating whether the unique steady state exists or not. Contraction mapping gives us a method or a tool to determine the combination of the operating parameters, the relationship between them. In the last class, we have formulated the basic theory of contraction mapping, how it has been formulated and the proof of the mathematical treatment of the idea that we already considered.

In the fragment of the last class, we have taken away particular example to apply the contraction mapping in order to determine the unique steady state. Now in this class, we will start with some more realistic chemical engineering system, where the contraction mapping will be utilized to determining the unique steady state. I will be considering a case of a chemical reactor, where the fermentation is going on to determine the unique steady state.

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Chemical Reactor.

Consider an catalyzed (by enzyme) fermentation Process. The Kinetics of the process is governed by Monod Kinetics. The reaction occurs in a CSTR with volume V , flow rate q . Feed concentration of reactant S is C_f . Reaction occurs isothermally. Irreversible reaction: $S \xrightarrow{\mu} P$

$$-\mu_A = \frac{K_1 C}{1 + K_2 C}$$

(i) Show the parameters of this system are $Da = \frac{K_1 V}{q}$; $\sigma = K_2 C_f$.

(ii) In order to have unique steady state $4 < \sigma < \infty$; $Da > 0.5 \left[(\sigma - 2) \pm \sqrt{\sigma^2 - 4\sigma} \right]$ with $\text{Min } Da = 1.0$

The first example will be a case of chemical reactor, we consider an enzyme catalyzed; this will be one of the most vivid example, where the contraction mapping will be utilized to obtain the condition on the operating parameters to get the unique steady state

by using contraction mapping. So, it is very important to follow up this example to a every detail.

Consider a catalyzed enzyme, catalyzed by fermentation process. The kinetics of the process is governed by Monod Kinetics. The reaction occurs in a C S T R, so we have talked about C S T R in the last class; it is a continuous start tank reactor, where the reactor is being start all the time and the feed comes into the system and goes out to the system. Since, if the reaction volume is appropriately started, it is assumed that the properties, the concentration and temperature in the reactor volume are uniform throughout. It is expected that whenever you will be drawing a product out of it; it will be having the same concentration and temperature that is existing inside the reactor. So that is the principle of continuous start tank reactor.

The reaction occurs in a C S T R with volume V and flow rate q . The feed concentration of reactant S , S is C_f ; reaction occurs isothermally. It is an irreversible reaction: the reaction is something like this, sub straight the monomer, the reactant gives the product with a weight constant, this is not a weight constant K_1 because it is a complicate Monod Kinetics. The rate expression is given as minus r_A is equal to $K_1 C$ divided by one plus K_2 times C .

Therefore, if this is the system, now the questions are (i) show the parameters - parameters are the combination of values of the operating conditions - parameters of these systems are Da that is called Damkohler number $K_1 V$ by q , σ K_2 time's C_f . We have to show that in order to have unique steady state this relationship should be the relationship of the parameters should exist; σ must be lying between 4 and infinity.

Damkohler number should be greater than 0.5σ minus 2 plus minus under root σ square minus 4 σ with minimum Damkohler number is 1. There is a minimum Damkohler number, the two parameters Damkohler number and σ they are basically the combination of the operating conditions. Damkohler number is multiplied by K_1 ; K_1 is basically one of the constant in the Monod Kinetics, V is the volume of the reactor, q is the flow rate.

Now, volume of the reactor and q ; the flow rate by which is getting into the system, these are under our control. These are the typical operating conditions, so we can have a selection on these. Similarly, K_2 times C_f ; K_2 may not be tuning for a particular

reaction, because it is fixed by the reaction kinetics, but feed concentration is in our control, so it is one of the major operating conditions.

Therefore, these two parameters: Damkohler, non dimensional parameter, Damkohler number and sigma must be obeying this relationship that sigma must be lying between 4 and infinity. Da has to be greater than this value in order to have a unique steady state for this particular problem.

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Solution:

Reactant balance equation at the Steady State

Rate of accumulation = Rate of in - Rate out + Rate of generation - Rate of consumption

$$qC_f - qC - (-r_A) \cdot V = 0$$

$$qC_f - qC - \frac{k_1 C}{1 + k_2 C} V = 0$$

$$C_f - C - \frac{(k_1 V/q) C}{1 + k_2 C} = 0$$

$$1 - X - \frac{(K_1 V/q) X}{1 + (K_2 C_f) X} = 0$$

$\frac{C}{C_f} = X$
non-dimensional concentration

Now, let us look into the solution of this problem. The solution goes like this; first, we write a material balance - species balance equation, it is basically reactant balance equation at the steady state.

Again, if we remember in the last class, probably we have developed for any balance equation; we write rate of accumulation is equal to rate of in minus rate out plus rate of generation minus rate of consumption. So, it is this general equation of balance equation is valid for every quantity, it may be a species balance, may be a concentration balance, may be a mass balance that mass accumulated in the system is equal to rate of mass going into the system minus rate of mass that is coming out of the system, rate of mass that is generated into the system and rate of mass is consumed in the system.

If it is a energy balance then it is rate of accumulation of it in a thermal energy is equal to rate of thermal energy going into the system minus going out of the system. If there is

some source term it will be generated, rate of generation should be included in a governing equation. If it is a dissipative system, then you have to write a rate of consumption term in your governing equation.

In our case, the material that is the rate of accumulation will be existing and rate of going into the material, the reactant that is going into the system that is there, going out of the system that is there, but there is no rate of generation of the reactant that is there in your system but, the reactant is continually consumed because of the reaction. So, rate of generation term will not be there and rate of consumption term will be there but, since we are talking about a steady state operation then rate of accumulation, which is time dependent part it will be not there, because at this the steady state is basically time independent portion of the profile of the operation.

Therefore, if you write the balance equation, so it becomes rate of material that is going into the system is q times C_f , q is the volumetric flow rate, so it has a unit of meter cube per second and C_f has a unit of concentration that is kg per meter cube, so q times C_f has a unit kg per unit time. So that is the rate of material of the substrate or the reactant that is going into the system minus q times C is the concentration of the reactant that is coming out of the system.

Interestingly, in case of CSTR, the same concentration exists into the reactor itself. So that is the material that is going into the system, that is the material that is coming out of the system, there is no generation of the reactant; on the other hand, reactant is basically getting consumed. So, this will be minus r_A times V so that will be equal to 0. This is the mass balance equation for the species in this particular problem.

Now, what we are going to do? We are going to substitute the expression of minus r_A by the Monod kinetics given in this problem. So, this becomes q times C_f minus q times C minus $K_1 C$ divided by $1 + K_2 C$ multiplied by V should be equal to 0, then we divide both set by q , so C_f minus C is equal to $K_1 V$ over $q C$ divided by $1 + K_2 C$.

Now, we make the concentration non dimensional by C by C_f and we call this quantity as non-dimensional concentration X , so this X is nothing but a non-dimensional concentration. This concentration is non-dimensionalized with respect to inlet concentration. So this will be $1 - X$ minus $K_1 V$ over q times X divided by $1 +$

we make this also non dimensional, so this will be $K^2 C_f$ multiplied by X . If you look into this equation; this equation, the first term is non-dimensional, the second term is non-dimensional and third term, it will be having, it will constitute of two parts numerator and the denominator.

If you look into the dimension of $K_1 V$ and q , so V by q is nothing but, a unit of second and K_1 will be having a unit of second inverse so this will be non-dimensional X is non-dimensional therefore, the denominator has to be non-dimensional. That means $K^2 C_f$, which K^2 will be having a unit of concentration inverse, so $K^2 C_f$ will be again a non-dimensional quantity.

Therefore, the parameter of this equation automatically comes out from the non-dimensionalization of the governing equation. That is in fact that is the aim of the first part of this question, you have to evaluate, you do not know, what are the non-dimensional parameters of a particular system of a mathematical model that will be the representing a particular chemical engineering system. So, first of all, you have to make it non-dimensional.

During the non-dimensionalization of the equation some of the parameters will be coming out automatically and these are the typical non-dimensional parameters, which are basically combination of the operating conditions, which will be relevant for this particular system. So, this is the method to identify the non-dimensional operating conditions or the non-dimensional parameters in a typical chemical engineering process.

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$Da = \frac{k_1 V}{q}; \quad \sigma = K_2 C_f.$
 $1 - x - \frac{Da x}{1 + \sigma x} = 0$
 $X = f(x)$
 $x \left[1 + \frac{Da}{1 + \sigma x} \right] = 1$
 $x \left[\frac{1 + Da + \sigma x}{1 + \sigma x} \right] = 1$
 $x = \frac{1 + \sigma x}{1 + Da + \sigma x}$
 LHS $\Rightarrow x = \frac{C}{C_f} \quad x \in [0, 1]$
 RHS $\Rightarrow \in [0, 1]$
 Governing eqn that mathematically represents this chemical engg. Process
 Isothermal $\Rightarrow$ X Heat bal.
 $\sigma, Da \rightarrow [0, \infty)$
 ≥ 0

We write down the non-dimensional parameters as Damkohler number equal to $K_1 V$ over q and σ is equal to K_2 times C_f . Let us write down the whole equation in its non-dimensional form $1 - x - Da \text{ times } x \text{ divided by } 1 + \sigma x$ is equal to 0.

Now, then what we will do? We rearrange this equation, therefore, this is a governing equation and since, it is an isothermal operation. This is the governing equation that mathematically represents this chemical engineering process. That is the isothermal enzyme catalyzed fermentation process, but since this process is isothermal, we need not to write the heat balance equation.

There is no need to write down the heat balance equation, **so we recast** so this governing equation in the form x is equal to f of x but, we have to remember, as we have seen in the last class, the casting of this equation is of extremely importance. So that you will be getting the domain of parameter on the left hand side must be the domain of the parameter in the right hand side. For example, if x lies in the domain 0 to 1 $f x$, the right hand side should also lies in the domain 0 to 1.

If x lies in the 0 to 1 and if $f x$ lies in the domain 0 to infinity then, the choice or rearrangement of this form x is equal to $f x$ is not appropriate. So, what is the appropriate form of x is equal to $f x$? Both the domain of left hand side and right hand side should be almost should be identical.

Therefore, we recast this equation in this form, we take one to the other side, so it will be $x + 1 + Da$ divided by $1 + \sigma x$ is equal to 1. So, $1 + \sigma x + 1 + Da$ plus σx should be is equal to 1, so x becomes $1 + \sigma x$ divided by $1 + Da + \sigma x$. So, this is the form x is equal to $f(x)$ for this particular problem.

Now, if you see the domain of the parameters of the variable the left hand side, what is x ? The x is nothing but c by C_f , so the maximum concentration of c should be C_f and the minimum should be 0, so x must be lying in the domain 0 to 1.

Now, if you look into the parameters σ and Da ; both σ and Da can be assuming any value in the domain 0 to infinity. So that is a generalized domain typically, they are all positive σ and Da both are positive. Depending on the parameters K_1 , K_2 , v and q , they will be assuming some values. So, generally you can say that σ and Da must be lying in the positive right half plane of the real axis. Therefore, σ and Da can be assuming any value.

If that is the case, if you look into the numerator, this is $1 + \sigma$ and on the other hand, if you look into the denominator, the numerator is $1 + \sigma x$ the denominator is $1 + \sigma x + Da$ some amount of positive real number. Therefore, this will be the numerator, the denominator will be always greater than numerator, whatever the value of x is or σ and Da is, the numerator is always less than denominator; if that is the case $f(x)$ will be a fraction always. So that means right hand side is also lying between domain 0 to 1. Therefore, this is an appropriate choice of x is equal to $f(x)$. This choice is very important and we have seen in the last class, so otherwise, you will be landing up with a wrong result.

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$$f(x) = \frac{1 + \sigma x}{1 + Da + \sigma x}$$

Definition: $d(f(u), f(v)) = \frac{f'(w)}{Z} d(u, v)$
 $Z = Z(w) \Rightarrow w \in [0, 1]$
 f is a contraction map if $|Z|_{\max} < 1$

$$f'(x) = \frac{d}{dx} \left[\frac{1 + \sigma x}{1 + Da + \sigma x} \right]$$

$$= \frac{\sigma}{1 + Da + \sigma x} - \frac{(1 + \sigma x) \sigma}{(1 + Da + \sigma x)^2}$$

$$= \frac{\sigma}{(1 + Da + \sigma x)} \left[1 - \frac{1 + \sigma x}{1 + Da + \sigma x} \right]$$

$$= \frac{\sigma Da}{(1 + Da + \sigma x)^2} \quad \checkmark$$

Now, we have identified what $f(x)$ is, so $f(x)$ is $1 + \sigma x$ divided by $1 + Da + \sigma x$. So, what we do? Now, if you look into the definition of contraction map, it said that metric between functions $f(u)$ and $f(v)$ should be equal to $f'(w)$ metric between u and v . This $f'(w)$, if you call this at Z which is a function of a continuous variable w , Z is a function of a continuous variable w lying in the same domain 0 to 1 ; it is lying in the same domain of x the original variable.

This map then, f is a contraction map if maximum value of z should be less than 1 . So then f will be depicting a contraction map since, we are assuming the maximum value of z is less than 1 that means any value of z below the maximum value will be basically less than 1 . Maximum value $Z_{\max} < 1$ condition ensures that any value of z will be less than 1 and it will be a fraction and this f will be a contraction map, so that is the idea therefore, we first evaluate $f'(x)$; $f'(x)$ is nothing but d/dx of $f(x)$. So, it will be $1 + \sigma x$ over $1 + Da + \sigma x$. We use the first function, differentiation of the first function and then differentiation of the second function. We take the numerator as the first one and denominator as the second one, so we differentiate the numerator in the first step, so it will be σ over $1 + Da + \sigma x$.

Next, we keep this as fixed $1 + \sigma x$ and differentiate one over $1 + Da + \sigma x$. Since, it is inverse, so there will be minus sign here, so it will be minus there multiplied by $1 + Da + \sigma x$ square of that.

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$f'(x)|_{x=w} = \frac{\sigma Da}{(1+Da+\sigma w)^2}$ $\sigma w < 1$

$= Z(w)$

Max Z $Z|_{\max} \Rightarrow W_{\max}=1$
 $\searrow$ $W_{\min}=0.$

$Z_{\max} = \frac{\sigma Da}{(1+Da)^2}$

For f' to be a contraction map.

$Z_{\max} < 1$

$\frac{\sigma Da}{(1+Da)^2} < 1$

Now, if you see that what is the implication of this is that so f prime x evaluated at x equal to w should be equal to z and we have talked about earlier and z is a function of continuous variable w lying in the domain 0 to 1. Therefore, remember that the next step is that we look into the maximum value of Z $Z_{\max}$. So, Z will be maximum under what condition? So that is our next step since, w maximum is equal to 1 and w minimum is equal to 0. Therefore, if we put since w is appearing only in the denominator of the expression of Z , if you put the maximum value of w here, it will be giving you the

minimum value of z . If you put minimum value of w in the denominator - since it is appearing in the denominator it will give you the maximum value of z .

So, Z maximum will be obtained when you put the w as the minimum value, at its minimum value. What is the minimum value of w ? Minimum value of w will be equal to 0. Therefore, Z max will be σD_a , we put w is equal to 0, so this becomes 1 plus D_a whole square. Now, we have already seen the condition of contraction mapping now. So, what is the condition for contraction mapping? For f to be a contraction map, the Z max should be less than 1. We put Z max to be less than 1 therefore, σD_a one plus D_a square should be less than 1. We simplify this equation and see what we get.

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$$\begin{aligned}
 & \frac{\sigma D_a}{(1 + D_a)^2} < 1 \\
 \Rightarrow & \sigma D_a < (1 + D_a)^2 = 1 + 2 D_a + D_a^2 \\
 \Rightarrow & D_a^2 + D_a(2 - \sigma) + 1 > 0 \\
 \Rightarrow & D_a^2 - D_a(\sigma - 2) + 1 > 0 \quad \text{quadratic in } D_a \\
 \Rightarrow & \frac{D_a^2}{2} - 2 D_a \frac{(\sigma - 2)}{2} + \left(\frac{\sigma - 2}{2}\right)^2 - \left(\frac{\sigma - 2}{2}\right)^2 + 1 > 0 \\
 \Rightarrow & \left(D_a - \frac{\sigma - 2}{2}\right)^2 > \left(\frac{\sigma - 2}{2}\right)^2 - 1 \\
 \Rightarrow & D_a - \frac{\sigma - 2}{2} > \pm \sqrt{\left(\frac{\sigma - 2}{2}\right)^2 - 1} \\
 \text{or, } & D_a > \frac{\sigma - 2}{2} \pm \frac{\sqrt{(\sigma - 2)^2 - 4}}{2} \\
 & > \frac{\sigma - 2}{2} \pm \frac{\sqrt{\sigma^2 - 4\sigma + 4 - 4}}{2}
 \end{aligned}$$

If we really simplify that equation, we will be getting σD_a divided by 1 plus D_a square of that less than 1. Therefore, σD_a should be less than 1 plus D_a square, so this will be equal to 1 plus 2 D_a plus D_a square. Therefore, this will be D_a square plus D_a 2 minus σ plus 1 should be greater than 0.

You are going to get this equation, so σ is typically a value in the positive domain, so you can write it as minus σ minus 2 plus 1 greater than 0. Now, let us try to solve this equation in terms of D_a , so it has become a quadratic in D_a . Therefore what we do? We do a mathematical analysis of this equation and see what we get. So, D_a square minus 2 times D_a times σ minus 2.

We multiply and divide by 2 and add sigma minus 2 divided by 2 square and subtract sigma minus 2 divided by 2 square 1 is there, keep the one should be greater than 0. We are trying to make a perfect square out of it therefore, we will be getting Da minus - considering these 3 terms - Da minus sigma minus 2 by 2 whole square should be greater than sigma minus 2 by 2 square minus 1.

Now, we have a perfect square on the left hand side and in the form y square minus m square in the right hand side. Just take the square root, you will be getting Da minus sigma by 2 sigma minus 2 by 2 should be plus minus root over sigma minus 2 by 2 square minus 1. You can take sigma term on the right hand side and come to the conclusion that Da should be greater than sigma minus 2 by 2 plus minus, simplify this equation, this will be 4 coming out of the root it will be 2. So, this will be sigma minus 2 whole square minus 4.

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$$Da > 0.5 \left[(\sigma - 2) \pm \sqrt{\sigma^2 - 4\sigma} \right] \checkmark$$

For a real solution,
 $\sigma^2 - 4\sigma > 0$
 $\sigma(\sigma - 4) > 0$
 $\sigma - 4 > 0$
 $\Rightarrow \sigma > 4$
 $4 < \sigma < \infty \Rightarrow \boxed{4 < \sigma < \infty} \checkmark$
 $Da_{\min} = 0.5 \times 2 = 1.0$

If you simplify this equation this will be sigma minus 2 by 2 plus minus sigma square minus 4 sigma plus 4 minus 4; this plus 4 minus 4 will be cancelled out and you will getting a very simple and amenable form of Da and then Da becomes greater than 0.5 sigma minus 2 plus minus under root sigma square minus 4 sigma.

This is one of the conditions on the parameters Da and sigma should satisfy in order to have a unique steady state on this particular problem. Similarly, **if you would like to have** for a real solution of the system, for a real solution the term within the under root, it has

to be positive otherwise, it will be an imaginary value. Therefore, another condition is $\sigma^2 - 4\sigma$ should be greater than 0. Solution of this will be σ into $\sigma - 4$ is greater than 0; σ should be greater than 0, but σ is always greater than 0 that will not give you any other interpretation. So, the limiting condition is $\sigma - 4$ should be positive, so $\sigma - 4$ should be positive that means σ should be greater than 4.

We get a bound on σ and in general, the maximum σ is lying between - it is lying on the positive real half plane up to infinity therefore, we can identify the domain of σ , the minimum value of σ should be 4 and the maximum value is infinity. So, σ must be lying in the domain 4 to infinity and we have obtained that. These two are the condition on the parameters, so what are the conditions on the parameters? The condition on the parameters is σ has to be greater than 4 and Damkohler number should be satisfying this equation, in order to have a unique steady state to this particular problem.

What is the minimum value of Damkohler number? If we put the value σ is equal to 4 there, we will be getting the minimum value of Damkohler number. So, Damkohler minimum will be turning out to be 0.5 into 2, so that will be equal to 1. So, this is a very interesting and a typical application of contraction mapping. We have seen that how contraction mapping can be utilized in case of enzyme catalyzed fermentation process. In order to obtain a unique steady state for this particular system, what will be the conditions on the parameter, we have to think of.

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#2 An enzymatically catalyzed reaction. Kinetics is governed by Monod's Kinetics.

$$-r_A = \frac{K_1 C}{(1 + K_2 C)^2}$$

Reaction is in a CSTR; $V = \text{volume}$, $q = \text{flow rate}$
Feed concentration $\rightarrow C_f$
Isothermal, irreversible reaction
 $S \rightarrow P$

Solution: Isothermal $\rightarrow$ No need to write energy balance.

We move to the next illustrative example. Next example of today's class is again - we consider an enzymatic catalyzed reaction and again, the kinetics is governed by Monod's kinetics, there is minus r of A is equal to $K_1 C$ divided by $1 + K_2 \text{ times } C$. Again, the reaction is occurring in a CSTR with volume V , flow rate q and feed concentration of reactant c_f .

Again, we are considering an isothermal irreversible reaction. Reactant gives the product and we have solved in the last problem as this is the governing equation of the reaction of the Monod's kinetic, but in this problem it will be slightly change; this will be K_1 minus r_A is equal to $k_1 C$ divided by $1 + K_2 C$ whole square. The only difference in this problem; this problem is almost identical of the previous problem, but the Monod Kinetics is different.

My intention is if we have the different kinetic rate of reaction then, what will be the typical bounds or the conditions on the operating variables, so that you will be getting the unique steady state for a particular system.

Now, keeping everything fixed, keeping all the parameters fixed by changing the reaction kinetics see how the relationship between the parameters will evolve in order to have a unique steady state in your particular example or a particular system.

Therefore, again in this problem the solution goes like this (Refer Slide Time: 40:21). Since it is isothermal, no need to write down the energy balance equation. It must be mentioned here that I will be taking very simple problems to illustrate the principles, but actually the problems may be quite complicated and the whole system may be non-isothermal then the equations may not be solved analytically in the class. So, one has to take request to the numerical techniques, so that thing must be kept in mind. We will be solving very simplified problem and try to illustrate the principle and how the solution changes by using the contraction mapping.

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Under Steady State, Species (reactant) balance equation.

$$qC_f - qC - \frac{K_1 C v}{(1 + K_2 C)^2} = 0$$

$C/q = X$

$$C_f - C - \frac{\left(\frac{K_1 v}{q}\right) C}{(1 + K_2 C)^2} = 0$$

$$1 - X - \frac{\left(\frac{K_1 v}{q}\right) X}{(1 + K_2 X)^2} = 0$$

$\frac{K_1 v}{q} = Da; \quad K_2 C_f = \sigma$

We write down the mass balance equation under the steady state. The species balance equation or that means basically, the reactant balance equation. So, this becomes q times C_f minus q times C minus $K_1 C$ times v divided by $1 + K_2 C$ whole square should be equal to 0. Again, the same principle, rate of accumulation is 0, q times C_f is the reactant coming into the system, q times C is the amount of reactant that is going out of the system per unit time minus the reactant that is consumed throughout the whole volume of the system. So, rate of reaction must be multiplied by the volume of the reactor, so we will be getting this equation. Again, we will be doing the something; we make the whole system non-dimensional. If you make the whole system non-dimensional, the following non-dimensional parameters will be evolving out of it.

We write c by C_f as x that is the non-dimensional concentration divide the whole equation by q . So, you will be getting c_f minus c minus $K_1 v$ divided by q times c plus $K_2 C$ square of that is equal to 0. Again, divide by c_f , so you will be getting 1 minus x minus $K_1 v$ over q times c by C_f , so that will be x plus $K_2 X$ square of that. So, this should be K_2 times C_f , we multiply and divide by C_f , there will be C_f here.

We have the evaluation of the non-dimensional parameters $K_1 V$ by q is nothing but Damkohler number K_2 times C_f is nothing but σ that whatever we have described earlier. There is a mistake here, if you divide by C_f this becomes 1 minus c by C_f , so it will be x naught one over x , so this will be x only.

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$$\begin{aligned}
 x + \frac{Da x}{(1+\sigma x)^2} &= 1 \\
 \Rightarrow x \left[\frac{Da + (1+\sigma x)^2}{(1+\sigma x)^2} \right] &= 1 \\
 \Rightarrow x &= \frac{(1+\sigma x)^2}{Da + (1+\sigma x)^2} = f(x) \checkmark \\
 x &\in (0, 1) \\
 \text{For } x=0 \Rightarrow f(x)|_{x=0} &= \frac{1}{Da+1} < 1 \\
 \text{For } x=1 \Rightarrow f(x)|_{x=1} &= \frac{(1+\sigma)^2}{Da + (1+\sigma)^2} < 1 \\
 f(x) &\in (0, 1)
 \end{aligned}$$

We rearrange this equation into cast it in the form of x is equal to $f(x)$. So, x plus Damkohler times x divided by 1 plus σx square is equal to 1 . Take x common, so it becomes 1 plus σx whole square Damkohler plus 1 plus σx square bracket end is equal to 1 .

Take the third bracket on the right hand side, so this becomes 1 plus σx square divided by Da plus 1 plus σx whole square, this is the form x is equal to $f(x)$ and we identify this is $f(x)$. As we have seen earlier that x lies in the domain 0 to 1 , so in this domain whatever the value of x , you can check it for x is equal to 0 that is the minimum value of x , what is the value of $f(x)$? For x equal to 0 , this will be 1 divided by Da plus 1 .

For x is equal to 1, this is the value of $f(x)$ at x is equal to 1, this will be $1 + \sigma$ divided by $D\alpha + 1 + \sigma$. Since, the parameters $D\alpha$ and σ are extremely high all real positive. In this case, 1 over $D\alpha + 1$, so it will be always less than 1 . In this case, this is $1 + \sigma$ divided by $D\alpha + 1 + \sigma$, so denominator is always greater than numerator, so this will be always less than 1 . In this case as well, f of x lying in the domain 0 to 1 . We have selected an appropriate map x equal to $f(x)$ and this has every quality to be qualified as a contraction map.

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Choice of $f(x)$ is appropriate
 $\Rightarrow$ it can be a well behaved contraction map.

$z = f'(w) \Rightarrow z|_{\max} < 1$, so that f is a contraction map.

$$f = \frac{(1+\sigma x)^2}{[D\alpha + (1+\sigma x)^2]}$$

$$f'(x) = \frac{2\sigma(1+\sigma x)}{D\alpha + (1+\sigma x)^2} - \frac{(1+\sigma x)^2 \cdot 2\sigma(1+\sigma x)}{[D\alpha + (1+\sigma x)^2]^2}$$

$$= \frac{2\sigma(1+\sigma x)}{[D\alpha + (1+\sigma x)^2]} \left[1 - \frac{(1+\sigma x)^2}{D\alpha + (1+\sigma x)^2} \right]$$

$$= \frac{2\sigma D\alpha(1+\sigma x)}{[D\alpha + (1+\sigma x)^2]^2}$$

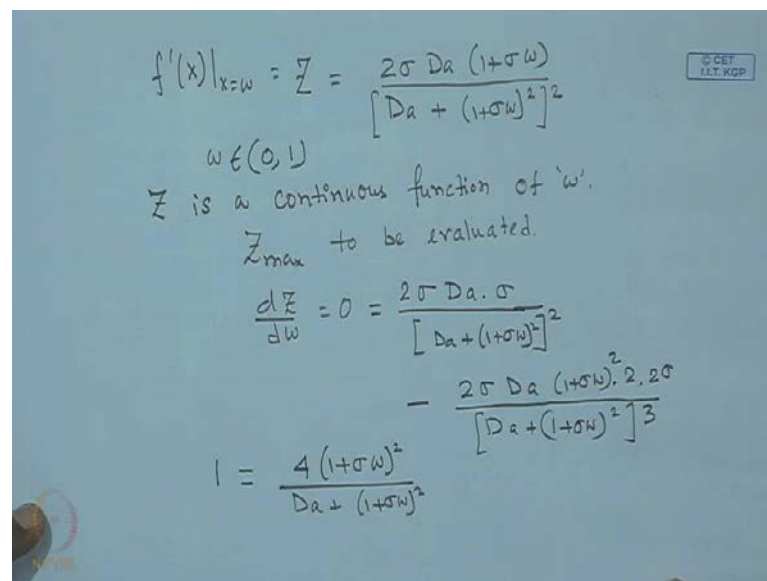
Next, if you remember the choice of $f(x)$ is appropriate and it can be a well behaved contraction map. In order to just find out the next of the steps, if you remember the next step is we find out f' prime w and we mark it as z , then we have to check that whether the maximum value of z should be less than 1 , so that f is a contraction map.

We follow the steps, first we evaluate f' prime x ; evaluate f' prime x at x equal to w but w is a variable lying in the same domain of x 0 to 1 then we evaluate z maximum and put z maximum less than 1 . Therefore, first we find out what is f' prime x ? $1 + \sigma$ square divided by $D\alpha + 1 + \sigma$ square. What is f' prime x ? Again, this numerator is as one function and denominator has the second function, so it will be $2\sigma(1 + \sigma x)$. This is the differentiation of the numerator, denominator remains as it is, then we differentiate the denominator. So, $1 + \sigma$ square remain as it is, the whole thing rest to the minus 1 .

On differentiation there will be minus sign here, then differentiation of this, so this will be this is constant no contribution from this term. From this term there will be contribution 2 comes from there, sigma comes from here, 1 plus sigma x and then denominator becomes a square, so 1 plus 1 plus sigma x square of that (Refer Slide Time: 48:36).

Now, let us simplify this equation, take 2 sigma 1 plus sigma x divided by Da plus 1 plus sigma x square common. So, it will be 1 minus 1 plus sigma x square divided by Da plus 1 plus sigma x square of that; one thing has taken so this square, out of this power 2 there will be only 1 that is left behind. On simplification 1 plus sigma x whole square in the numerator will be cancelled out, so what we will be getting only as 2 sigma Da 1 plus sigma x divided by Da plus 1 plus sigma x square of that then whole square. So that gives the expression of prime x.

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$$f'(x)|_{x=w} = Z = \frac{2\sigma Da (1+\sigma w)}{[Da + (1+\sigma w)^2]^2}$$

$w \in (0,1)$
 Z is a continuous function of 'w'.
 $Z_{\max}$ to be evaluated.

$$\frac{dZ}{dw} = 0 = \frac{2\sigma Da \cdot \sigma}{[Da + (1+\sigma w)^2]^2} - \frac{2\sigma Da (1+\sigma w)^2 \cdot 2 \cdot 2\sigma}{[Da + (1+\sigma w)^2]^3}$$

$$1 = \frac{4(1+\sigma w)^2}{Da + (1+\sigma w)^2}$$

Next, we evaluate f prime x at x is equal to w. We evaluate that f prime x evaluated at x is equal to w and we called that as z and this becomes 2 sigma Da 1 plus sigma w divided by Da plus 1 plus sigma w square, square of that. Now, if you remember that we have already seen that what is the value of w; w is again in a running variable, it is a variable lying in the same domain of x from 0 to 1. Therefore, z is a continuous function of w.

In order to have this z to be less than 1, we should consider what is the maximum value of z ; if that is less than 1 then all the values will be less than 1. Next we evaluate $Z_{\max}$; $Z_{\max}$ to be evaluated, how $Z_{\max}$ will be evaluated? $Z_{\max}$ will be evaluated since z is a continuous function of w . We use dz/dw is equal to 0, we evaluate dz/dw and put it equal to 0 that will give you the maximum value of z . If you do that so it will be 0 is equal to $2 \sigma Da$ times σDa plus 1 plus σw square, square of that minus one more differentiation for the denominator, the numerator remains constant. So, $2 \sigma Da$ 1 plus σw that is present there.

Next we will be getting 2 times $2 \sigma Da$ and one more 1 plus σw will be coming, so this will be there will be square of that divided by Da plus 1 plus σw square. Since, there is a differentiation this will be minus 2, so after differentiation it will be minus 3, so it will be denominator it will be cube. We put it equal to 0 so after doing all these simplification, I am just omitting one more step and writing the expression 4 into 1 plus σw square divided by Da plus 1 plus σw square.

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Handwritten derivation on a blue background:

$$3(1+\sigma w)^2 = Da$$

$$\Rightarrow \frac{(1+\sigma w)^2}{1+\sigma w} = \frac{Da}{3}$$

$$\frac{1+\sigma w}{1+\sigma w} = \sqrt{\frac{Da}{3}}$$

$$Z_{\max} = \frac{2 \sigma Da \sqrt{\frac{Da}{3}}}{(Da + \frac{Da}{3})^2}$$

$$= 2 \sigma \cdot \sqrt{\frac{Da}{3}} \cdot \frac{9}{16 Da^2}$$

$$= \frac{9}{8\sqrt{3}} \frac{\sigma}{\sqrt{Da}}$$

For contraction mapping

$|Z_{\max}| < 1$
 $\frac{\sigma}{\sqrt{Da}} < \frac{8\sqrt{3}}{9}$

Therefore, we will be getting this equation 1 plus; the equation that we will be getting 1 plus σw square multiplied by 3 is equal to Damkohler number, so 1 plus σw square will be Da by 3. At this value of 1 plus σw whole square it becomes Da by 3.

So, $1 + \sigma w$ is nothing but Da by 3 under root. Here, at this condition z becomes maximum. What is the value of $Z_{\max}$? Maximum value of z is that wherever in the expression of z we have $1 + \sigma w$ going to represent by root over Da by 3 .

If that is the case, so this becomes $2 \sigma Da$ root over Da by 3 divided by Da plus 1 plus σw whole square, so it will be Da by 3 square of that. So, what we will be getting is that $2 \sigma Da$ root over Da by 3 multiplied by - this will be $3 + 1$ so it will be 4 by 3 , so 9 by $16 Da$ square in the denominator. So, $1 Da$ $1 Da$ will be cancelling out, so will be 2σ , so 9 by 8 root 3σ by root over Da , so one Da will be here root over Da , there σ by root over Da . We will be having square there, so that is fine, this 9 is there, so this will be 9 by 8 by root 3σ by root over Da .

Now for contraction mapping, our condition is that $Z_{\max}$ should be less than 1 therefore, σ by root over Da should be less than 8 root 3 divided by 9 . **This is the condition of contraction map** this is the condition for this particular problem where we will be having existence of unique steady state. Root 3 is around 1.732 , so this will be this value will be 8 into 1.732 , it will be a value around 14 divided by 9 . So, it will be around **0.7** 0.8 so, σ by root over Da should be less than 0.8 or so. So that is the condition of the operating variables σ and Da should satisfy in order to have a unique steady state for this particular problem.

Again, this example demonstrates how the contraction mapping would be utilized to find out the unique steady state in any chemical engineering system. We stop here, in the next class, we will be taking up one more example of contraction mapping, so the calculations and the procedure becomes absolutely clear to all of you and then, we will move to the next topic. Thank you very much.