Advanced Process Dynamics

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Lecture 01

Introduction and motivation

About the course

Part 1: Analysis of dynamics of linear systems in state-space domain

- Autonomous first order systems
- Phase portraits of higher order systems
- Non-autonomous higher order systems

Part 2: Analysis of dynamics of non-linear systems in state-space domain

- Non-linear first order systems
- Higher order non-linear systems
- Discrete systems, bifurcation and chaos

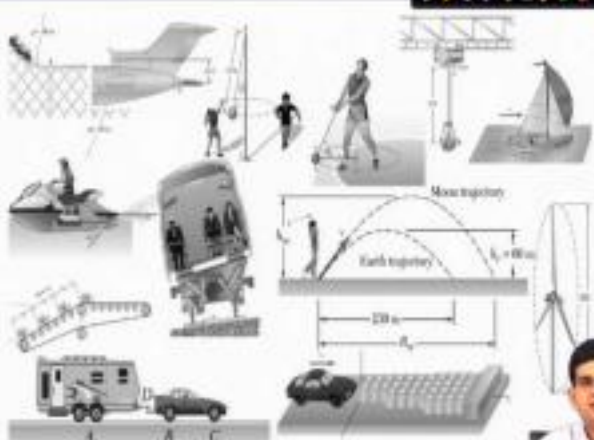
Part 3: Transform domain analysis of linear systems

- Response to ideal forcing functions
- Different types of transfer functions
- Multiple input - multiple output systems

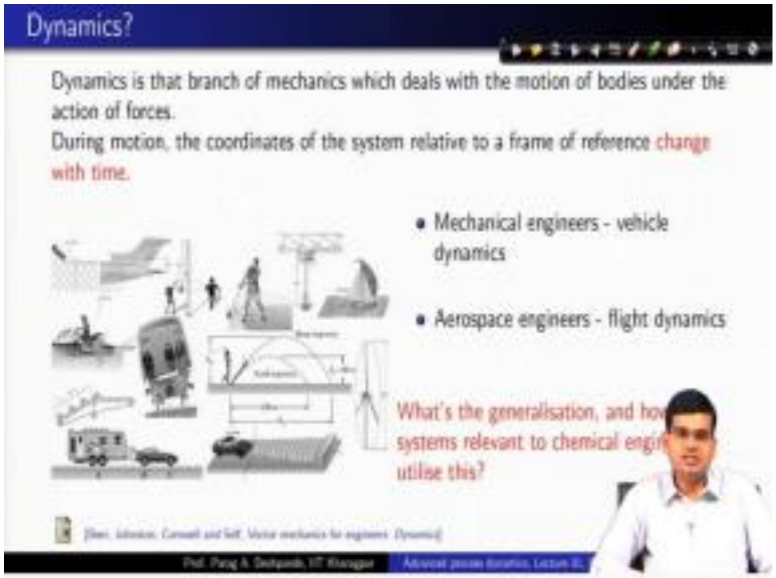
Part 4: Tranform domain analysis of discrete-time systems

- Introduction to Z-transforms
- Response of discrete-time systen
- Stability analysis of discre

Dynamics?



[Beer, Johnston, Cornwell and Self. Vector mechanics for engineers: Dynamics]


Dynamics?
Dynamics is that branch of mechanics which deals with the motion of bodies under the action of forces.
During motion, the coordinates of the system relative to a frame of reference change with time.
Mechanical engineers - vehicle dynamics
Aerospace engineers - flight dynamics
What's the generalisation, and how systems relevant to chemical engi utilise this?
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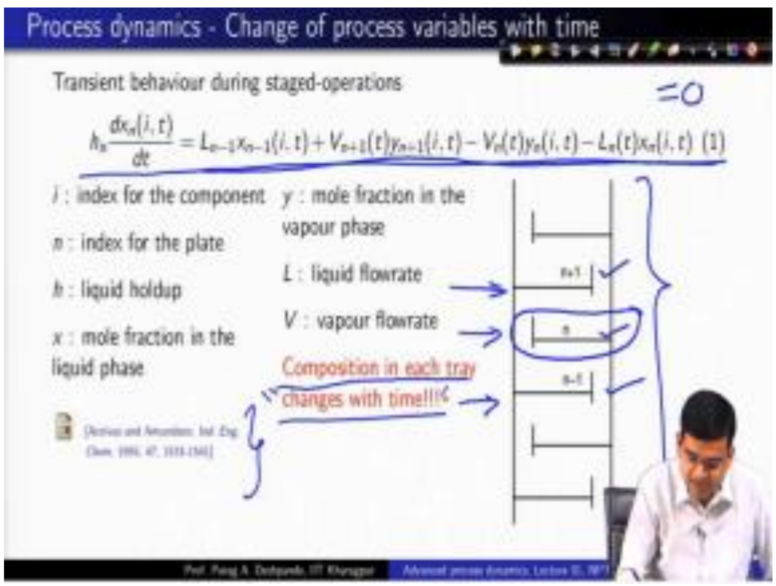
Process dynamics - Change of process variables with time
Transient behaviour during staged-operations
=0
$h_n \frac{dx_n(i,t)}{dt} = L_{n-1}x_{n-1}(i,t) + V_{n+1}(t)y_{n+1}(i,t) - V_n(t)y_n(i,t) - L_n(t)x_n(i,t)$ (1)
i : index for the component
n : index for the plate
h : liquid holdup
x : mole fraction in the liquid phase
y : mole fraction in the vapour phase
L : liquid flowrate
V : vapour flowrate
Composition in each tray changes with time!!!
n+1
n
n-1
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Process dynamics - Change of process variables with time

Transient operation of a jacketed CSTR

$$\frac{dC}{dt} = \frac{F}{V}(C_f - C) - r \quad (3)$$

$$\frac{dT}{dt} = \frac{F}{V}(T_f - T) + \left(\frac{-\Delta H}{\rho c_p}\right) r - \frac{UA}{V\rho c_p}(T - T_j) \quad (4)$$

F : volumetric feed rate

C_f : concentration of the reactant in the feed

T_f : temperature of the feed

C : concentration of the reactant in the reactor

T : temperature of the reaction mixture

F_j : volumetric flowrate of the heating/cooling fluid

T_j : temperature of the heating/cooling fluid

V : volume of the reactor

r : rate of reaction

Concentration and temperature in the reactor change with time!!!

[Bequette, Process dynamics: Modeling, analysis and simulation]

Process dynamics - Change of process variables with time

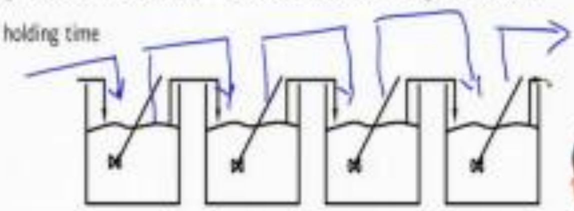
Transient operation of n cascade CSTRs with reversible series reactions

$$\frac{dc_1(1)}{dt} = -\left(k_1 + \frac{1}{\theta}\right)c_1(1) + k_1' c_2(1) + \frac{1}{\theta}c_1(0) \quad (2)$$

$c_i(n)$: concentration of the i^{th} species in the n^{th} reactor

$c_i(0)$: concentration of the i^{th} species in the feed entering the first tank

θ : holding time



Concentrations in the reactors change with time!!!

Some definitions

Dynamical variable

The time-dependent variable whose time rate of change is described by the model equation is called the dynamical variable.

$$h_n \frac{dx_n(i,t)}{dt} = L_{n-1}x_{n-1}(i,t) + V_{n+1}(t)y_{n+1}(i,t) - V_n(t)y_n(i,t) - L_n(t)x_n(i,t) \quad (1)$$

$$\frac{dc_1(1)}{dt} = -\left(k_1 + \frac{1}{\theta}\right)c_1(1) + k_1' c_2(1) + \frac{1}{\theta}c_1(0) \quad (2)$$

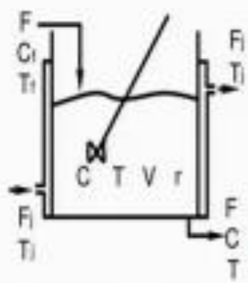
$$\frac{dC}{dt} = \frac{F}{V}(C_f - C) - r$$
$$\frac{dT}{dt} = \frac{F}{V}(T_f - T) + \left(\frac{-\Delta H}{\rho c_p}\right)r - \frac{UA}{V\rho c_p}(T - T_j)$$

Some definitions

Order of a system - Old definition

Order of a system is the order of the ODE that models the system.

$$\frac{dC}{dt} = \frac{F}{V}(C_f - C) - r$$
$$\frac{dT}{dt} = \frac{F}{V}(T_f - T) + \left(\frac{-\Delta H}{\rho c_p}\right)r - \frac{UA}{V\rho c_p}(T - T_j)$$



Two first order ordinary differential equations. So what's the order?

Some definitions

Order of a system - New definition

Order of a system is the *"number of first order"* ODE's that model the system.

$$a_2\frac{d^2x}{dt^2} + a_1\frac{dx}{dt} + a_0x = bf(t) \quad -(1) \leftarrow \text{one } 2^{nd} \text{ order ODE}$$

$$\frac{dx}{dt} = y \text{ (say)} \quad -(2) \leftarrow \text{First } 1^{st} \text{ order ODE}$$

$$a_2\frac{dy}{dt} + a_1y + a_0x = bf(t)$$

$$\Rightarrow \frac{dy}{dt} = -\frac{a_0}{a_2}x - \frac{a_1}{a_2}y + \frac{b}{a_2}f(t) \quad -(3) \leftarrow \text{second } 1^{st} \text{ order ODE}$$

two 1^{st} order ODE's

Some definitions

Linear system

A system is said to be a linear system if its governing dynamical equations are linear.

Principle of linearity

If $\tilde{L}$ is an operator in a linear vector space and $\underline{u}$ and $\underline{v}$ are the two vectors in the linear vector space then the operator $\tilde{L}$ is said to be linear if it satisfies the following:

$$\tilde{L}(\underline{u} + \underline{v}) = \tilde{L}(\underline{u}) + \tilde{L}(\underline{v}) \quad (5)$$

$$\tilde{L}(\alpha\underline{u}) = \alpha\tilde{L}(\underline{u}) \quad (6)$$

where α is an element of the field over which the vector space is defined.

A system which does not follow the above principle of linearity is referred to as a non-linear system.

[Suggested further reading: Strang, Introduction to linear algebra]

Some definitions

Linear system

A system is said to be a linear system if its governing dynamical equations are linear.

$$\frac{d^2x}{dt^2} + ax = 0 \qquad -(1)$$

$$\hat{L} = \frac{d^2}{dt^2} + a$$

$$\hat{L}x = \left(\frac{d^2}{dt^2} + a\right)x = \frac{d^2x}{dt^2} + ax$$

$$\hat{L}x = 0$$

Some definitions

Linear system

A system is said to be a linear system if its governing dynamical equations are linear.

$$\frac{d^2x}{dt^2} + ax = 0 \qquad -(1)$$

Let x_1 and x_2 be two solutions of Eq^n (1)

$$\hat{L}x_1 = \frac{d^2x_1}{dt^2} + ax_1$$

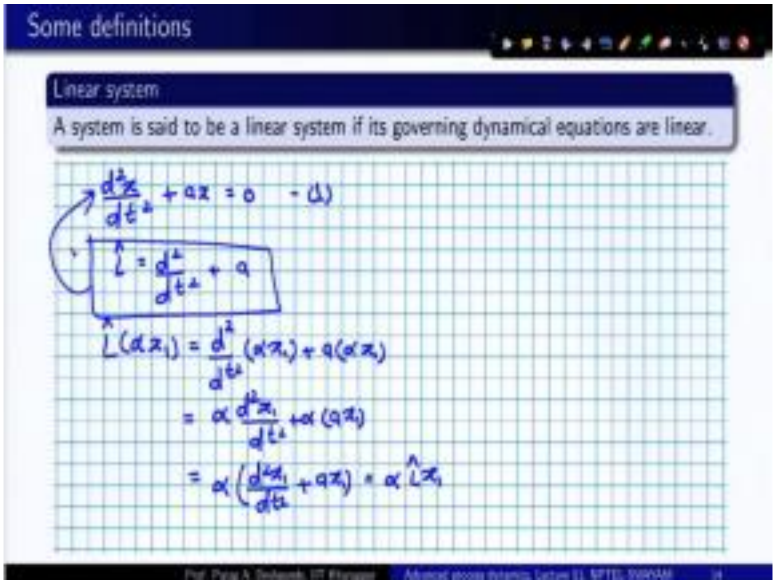
$$\hat{L}x_2 = \frac{d^2x_2}{dt^2} + ax_2$$

$$\hat{L}(x_1 + x_2) = \left(\frac{d^2}{dt^2} + a\right)(x_1 + x_2)$$

$$\hat{L}(x_1 + x_2) = \frac{d^2x_1}{dt^2} + \frac{d^2x_2}{dt^2} + ax_1 + ax_2$$

$$= \left(\frac{d^2x_1}{dt^2} + ax_1\right) + \left(\frac{d^2x_2}{dt^2} + ax_2\right)$$

$$= \hat{L}x_1 + \hat{L}x_2$$



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Hello, and welcome to this online course on Advanced Process Dynamics. I am P.A. Deshpande from the Department of Chemical Engineering at IIT, Kharagpur. And over the next 12 weeks, we will engage ourselves in learning some new and advanced techniques with special relevance to process industries. We will also take examples from other domains like mechanical engineering, aerospace engineering, biotechnology, etc. But the prime focus will be on process engineering applications.

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So, before I start, let me give a brief overview of the course structure. Throughout this course, I will be accompanied by two of my graduate students: Abhishek and Mayalekshmi. We will learn some advanced techniques. So, you will soon realize what do I mean by advanced, when I go through the course contents. The prerequisite for the course is an elementary course on Process Dynamics and Control.

The general UG curriculum of chemical engineering introduces the students to process dynamics and control, but the course also comes with different names such as process instrumentation and control or control engineering. We will be starting every topic with a mathematical technique, and then subsequently we will be taking an example from process industry.

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So, therefore, it would be highly desirable if you have at least one of the courses on linear algebra or ordinary differential equation and transform calculations. So, we will meet every week for five times, every lecture would be of 30 minutes duration and we will complete the course in the next 12 weeks.

So, what we will do today is I will formally define the various terms which we will be using repeatedly in this course over the next few -- over the next 12 weeks, in fact. So, let us start with the formal definition of process dynamics. The process dynamics involves the dynamics of change, and it can be analysed in two different methods, it can be analysed in state space domain or it can be analysed using transform domain.

So therefore, the first two parts of the course will involve the analysis of processes in state space domain, followed by analysis of processes in transform domain. Processes in industries are both linear as well as nonlinear. And we will do the analysis of processes in state space domain as well as in transform domain which involved both linear as well as nonlinear processes.

Further, especially with the introduction of computers for control of processes, several processes are no more in continuous domain, but they take place in discrete domain. So, we will also analyse how to do the analysis of process dynamics in discrete domain. So, these are the four different parts of the course that we would be covering in the next 12 weeks.

(Refer Slide Time: 03:52)

So, let us start the course. And let us first ask ourselves the question that what is the meaning of dynamics? So, let us forget about process dynamics. And let us first see what is the meaning of dynamics? I am confident that you have come across the word, dynamics for the first time in your high school physics, where you learned about statics and dynamics as two major branches of mechanics.

I am also confident that you must have taken one or the other flavour of Engineering Mechanics courses in your engineering curriculum. And there also you must have been introduced to the concept of dynamics. In fact, I made this collage to remind yourself of various problems or type of problems that you must have solved using one famous book by Beer and Johnston. And what do we actually understand by dynamics when we refer to the word dynamics in say pure physics or also engineering mechanics?

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So, the term dynamics refers to that branch of Mechanics, which deals with the motion of bodies under the action of forces. So, what is the key word here? The key word is that the motion of the bodies takes place and the coordinates of the bodies change with time. So, the key word is change with time.

Now, if you were a Mechanical engineer, you would have used this concept by applying the concepts of dynamics to the motion of, say vehicles. And that is what gives rise to the branch of what is called Vehicle Dynamics. Similarly, Flight Dynamics is studied by Aerospace engineers, where they learn about how to make an aircraft air bound safely and also land it safely. And in both the cases, what happens is that the coordinates of the vehicle or the aircraft changes with time.

Now, the question is, how can we perhaps use similar concepts or perhaps the same concepts in Process Engineering applications? The answer comes from the phenomenal work of a Mathematician Henri Poincare, who developed the theory of dynamical systems, which was nothing but the analysis of ordinary differential equations.

What Henri Poincare showed is that even simplest of the ordinary differential equations can have very, very complex behaviour, as you change the state of the system, as you change the parameters of the system. And Chemical engineers then realized that we can in fact, use the concept of dynamical systems which exist in Mathematics in case of process industries as well. So, what is the difference between dynamics in general and process dynamics? Process dynamics deals with the systems which undergo change with time.

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So, we can take several of such examples, one of the examples can be the staged operation of for example, a distillation column. So, what you can see here is a distillation column with different number of trays. And let us consider three trays indexed as n+1, n and n-1. You must have been taught in your mass transfer or separation process courses that you can do a mole balance over one particular plate.

And what you can see on the right-hand side of this equation is the mole balance and you used to equate it simply to zero to determine how much of a particular component leaves one tray to go to the upper tray or the liquid phase to go to the downward tray and so on. But there was an inherent assumption that the process was taking place at steady state. But imagine that you have started your distillation column and it is going to take some time for the system to reach the steady state where changes do not take place with time, everything remains constant.

Now, the question is what happens during the time that you start your operation and then you go and reach the steady state. So, that is a transient-dynamics that you need to capture. And that is given by this equation, which you can see here on the screen. I have taken this example directly from the work of Acrivos and Amundson. And the terms which you can see here have been used directly from the ones reported in the paper. So, in case you want to refer to the original work, you can actually look at this equation and refer to the original work.

The equation is very simple. It is simple transient mass balance equation. So, this is a dynamical system because the composition in each tray changes with time. So, change with time is important term here, and therefore, this is a dynamical system.

(Refer Slide Time: 09:30)

Let us look at another example. So, imagine that you have a CSTR and you operate the CSTR under transient conditions. So, what is going to happen? Instead of one equation, you are going to now have two equations because the concentration of the species is going to change with time. So, is the temperature of the species going to change with time.

So, now you have two equations, in both the cases what you see is that the equations involve change of concentration and change of temperature with time. So, therefore, all those traditional, a conventional CSTR is meant to be operated at steady state, but before the steady state is reached the system experiences transients and you can solve these model equations by analysing the dynamics of the system and you can come to know how quickly or how slowly does the system reach the steady state condition.

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Finally, we can take one more example and take the example of CSTRs in series. So, again you have transient operation of n cascade CSTRs with reversible series reactions. It is not very difficult to see from the schematic that you have a feed to this CSTR, you have a feed to the CSTR and the reactant concentration with some initial concentration goes to the first CSTR. From the first one, it moves to the second one and so on.

Again, during the steady state operation, you would expect the model equations to be independent of time, but, when transient operation takes place, the concentrations of the species inside the CSTR changes with time. And therefore, you need to understand the dynamics of the system. So, therefore, we come across a lot of process engineering applications, where the properties of or the variables associated with the system change and the change happens in time. And dynamical systems or process dynamics is the study of such systems.

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So, let us define formally what is the meaning of dynamical systems. So, a dynamical system is defined as a system which has at least one variable which changes with time, which is a function of time. So, these are all the model equations which we saw in the past three cases. And what we see is that in all the three cases we have the system which changes with time.

So, therefore, the case of a distillation column which is operating under transient conditions or CSTRs in series or a non-isothermal operation of a CSTR, all of these are the cases where the system changes with time and therefore, you define such systems as dynamical systems. Now, what is the meaning of a dynamical variable. The dynamical variable is a variable which changes with time and for such variables, the time rate of change is described by the model equation.

So, in these four equations, you see that there are quantities which are highlighted in red, you have x of n which is the molar composition over any tray of any component, then you have C_i of 1 which is the concentration of the i^{th} component in a given reactor, then for the case of CSTR you have the composition as well as temperature which change with time. And in all of these cases, what you see is that you have identified a variable which changes with time and such a variable is called the dynamical variable.

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Now, we can define traditionally the order of a system. In your undergrad process dynamics and control course, you must have studied the definition of an order of a system as the order of the ordinary differential equation that models the system. So, for example, if you take a manometer and do the dynamics of the motion of the liquid, the model equation comes from the Newton's second law.

And since Newton's second law is second order, you say the order of the system or the order of dynamics of liquid level in a manometer is two. But now, we have a problem, what you see here is that for the case of a CSTR, you have two equations and each equation is a first order equation. And if such is the case, that you have two first order ordinary differential equations, then what is the order of the system?

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So, now we define a new definition of the order of the system as the number of first order equations, which are present in the system. So, order of a system will now be the number of first order ODEs that model the system. And is there a correspondence between the older definition and the new definition?

Well, we can establish that, let us consider a general second order ODE. So, the equation is

$$a_2 \frac{d^2x}{dt^2} + a_1 \frac{dx}{dt} + a_0 x = b\, f(t) \qquad \ldots\ldots\ldots\ldots\ldots (1)$$

So, this is my general second order ODE and let us say this ODE governs the system. So, the system is a second order system, following our previous definition.

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So, now, what I do is I define a new variable

$$\frac{dx}{dt} = y \qquad \ldots\ldots\ldots\ldots\ldots\ldots (2)$$

Say this is the new variable. So, what I will do is, I will substitute $\frac{dx}{dt} = y$ in equation one so, I get,

$$a_2 \frac{dy}{dt} + a_1 y + a_0 x = b\, f(t)$$

And this can be rearranged as:

$$\frac{dy}{dt} = -\frac{a_0}{a_2} x - \frac{a_1}{a_2} y + \frac{b}{a_2}\, f(t) \qquad \ldots\ldots\ldots\ldots\ldots\ldots.. (3)$$

So, let us now analyse what we have done. I had previously one second order ODE which govern my system and therefore, the system was second order. And I have converted it to two first order ODEs. So, this is the first, first order ODE and this is the second first order ODE, which means all together I have two first order ODEs, which means that it is possible for me to convert any second order ODE to a set of two first order ODEs and by induction I can say that I can convert any nth order ODE to n first order ODE. So, therefore, our new definition that the order of a system is equal to the number of first order ODE is that model the system is in fact consistent with our previous definition.

So, now, let us take one more concept and define what a linear system is? So, we will be dealing with linear as well as nonlinear systems, we need to first define what a linear system is. So, a linear system is defined as the one whose governing dynamical equations are linear now, this is a very recursive definition. We are defining a linear system as a system whose dynamical equations are linear.

So, we need to properly define what is the meaning of linearity, how do you say that a system is that the governing equations themselves are linear. So, according to the principle of linearity the first thing that you need to do is you need to identify the corresponding operator for your equation.

So, our equations would be ordinary differential equations. And for every equation, for every ODE, you will need to determine the corresponding operator. And if the corresponding operator is linear, then your system is linear. Again, what is the meaning of the term that the corresponding operator is linear? Well, it needs to satisfy two conditions given by equations five and equation six.

Let us see, what is the meaning of these two conditions. So, let us imagine that I have identified $\hat{L}$

as the operator, we will very quickly see how do I identify the operator, but, at this point of time, let us see that I have identified an operator and that operator lies in a linear vector space whose two elements u and v are known to me. So, u and v are the two elements of a linear vector space and $\hat{L}$ is defined in that linear vector space.

Then, the system -- the operator $\hat{L}$ is said to be linear, if

$$\hat{L}(u+v) = \hat{L}(u) + \hat{L}(v)$$

And if α is any member of the field over which the vector space is defined then,

$$\hat{L}(\alpha u) = \alpha\, \hat{L}(u)$$

(Refer Slide Time: 21:57)

So, let us quickly look into how we actually can establish this. So, let me say that I have a model equation which goes like this,

$$\frac{d^2x}{dt^2} + ax = 0 \qquad \ldots\ldots\ldots\ldots\ldots.. (1)$$

So, as I said I need to identify the operator. So, let us see if I write this and you get convinced that this is the operator,

$$\hat{L} = \frac{d^2}{dt^2} + a$$

So, $\hat{L}$ is an operator which means that I will have a quantity over which $\hat{L}$ would be operating. So,

$$\hat{L}x = \left(\frac{d^2}{dt^2} + a\right)x$$

And what is the meaning of operating on x? So, I have second order derivative here, which means, I will have $\frac{d^2x}{dt^2} + a$ is simply a multiplication operator which means, I will have ax here. And my equation would be,

$$\hat{L}x = 0$$

So, I have done the first step that is the identification of operator.

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So, let us see I have,

$$\frac{d^2x}{dt^2} + ax = 0 \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots (1)$$

Now, I need to verify whether the principles of linearity hold true. So, I say that let x_1 and x_2 be two solutions of equation one, this is my equation one. So, since I have a linear, if I have a linear system the solutions would lie in the linear vector space.

So, if the two solutions are any two solutions are x_1 and x_2 then I will have,

$$\hat{L}\,x_1 = \frac{d^2x_1}{dt^2} + ax_1$$

$$\hat{L}\,x_2 = \frac{d^2x_2}{dt^2} + ax_2$$

Now according to my first property, what I should do is I should operate $\hat{L}$ on $x_1 + x_2$.

So, what would this be?

$$\hat{L}\,(x_1 + x_2) = \frac{d^2x_1}{dt^2} + \frac{d^2x_2}{dt^2} + ax_1 + ax_2$$

$$\hat{L}\,(x_1 + x_2) = \left(\frac{d^2x_1}{dt^2} + ax_1\right) + \left(\frac{d^2x_2}{dt^2} + ax_2\right)$$

So, my property of -- first property of linearity is indeed satisfied.

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Let us go and look into the second property. So, my equation is

$$\frac{d^2x}{dt^2} + ax = 0 \qquad \text{………………..} (1)$$

And my operator is

$$\hat{L} = \frac{d^2}{dt^2} + a$$

According to my second property, if α is any member of the field over which the solution space is defined, then, if I operate $\hat{L}$ (αx_1), where x_1 is any solution, then what is going to happen is that,

$$\hat{L}(\alpha x_1) = \frac{d^2}{dt^2}(\alpha x_1) + a(\alpha x_1)$$

So, I can do a quick rearrangement, this would be:

$$\hat{L}(\alpha x_1) = \alpha \frac{d^2 x_1}{dt^2} + \alpha(ax_1)$$

$$\hat{L}(\alpha x_1) = \alpha\left(\frac{d^2 x_1}{dt^2} + ax_1\right)$$

And what is this equal to?

$$\hat{L}(\alpha x_1) = \alpha \hat{L} x_1$$

So, the second property is also satisfied and I see that

$$\hat{L}(x_1 + x_2) = \hat{L}(x_1) + \hat{L}(x_2)$$

and

$$\hat{L}(\alpha x_1) = \alpha \hat{L} x_1$$

So, therefore, the operator here $\hat{L}$ corresponding to this equation in fact is a linear operator and therefore, the equation also is a linear equation.

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So, now, final question which arises in our mind is that, how to analyse the dynamics or analyse the dynamical systems. As I made a mention in the during the beginning of the lecture, that there are basically two broader ways of analysis one is called the state space domain analysis, the other one is called the transform domain analysis.

So, when do we do state space domain analysis and when do we do transform domain analysis? Typically, most chemical plants these days operate 24x7 on a continuous mode of operation. So, if a plant operates for say six months continuously and during that operation there would be small fluctuations in the process variables and you will have control system implemented in it for maintaining the process variable.

But then the question is that if you know that this is my say the level of temperature which I need and the temperature falls down by 100^0C. So, I need to understand the dynamics of my system between two steady states. This is the first initial steady state which you want, the system has gone to the lower steady state, you probably would like it to come back to the original steady state and so on and so forth.

When you want to do the analysis of the system between the known steady states, then you do the analysis in transform domain and this is typically what is taught in the undergrad curriculum. But then, when you design a process, you would like to know what all can happen to my system. Will my system -- what is the maximum temperature for example, which can -- which my system can reach? Will my system be able to -- system parameters be able to afford that condition of temperature, pressure and so on. So, you are not merely focusing on the dynamics between two steady states, but you are trying to understand the dynamics between, understand the dynamics, which is in every post possible parameter space domain. In such a case, you use the state space domain analysis.

We will begin our lecture by now, we will begin our course, by state space domain analysis. We will focus on the analysis of the systems using various concepts which arise during the state space domain analysis. And then, during the latter part of the course, we will resort to the transform domain analysis. So, we will stop here today and we meet tomorrow with the new topic of analysis in state space domain. Thank you.