Process Dynamics and Control

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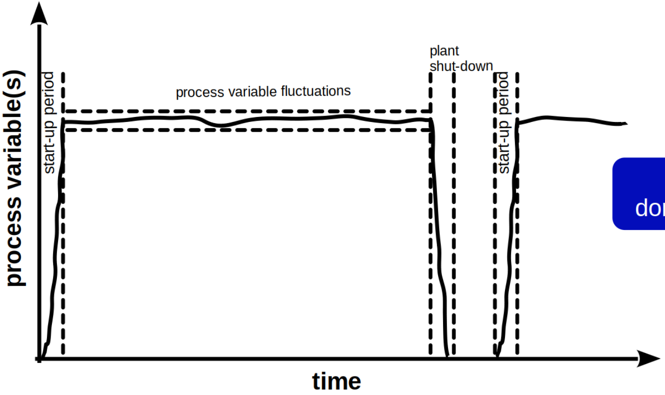
- [Bequette, *Process Dynamics: Modeling, Analysis, and Simulation*]
- [Ogunnaike and Ray, *Process Dynamics, Modeling, and Control*]
- [Stephanopoulos, *Chemical Process Control*]

Reasons and approaches to study process dynamics

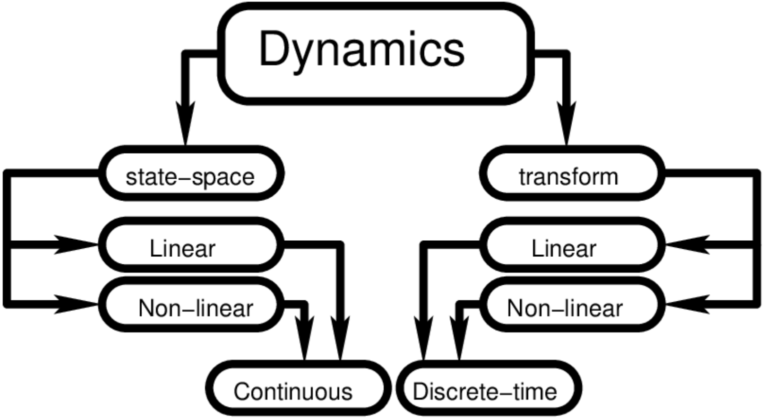
Most chemical plants operate 24 $\times$ 7 in a continuous mode of operation with periodic shut-down for maintenance.

state-space domain analysis



transform domain analysis

Reasons and approaches to study process dynamics



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

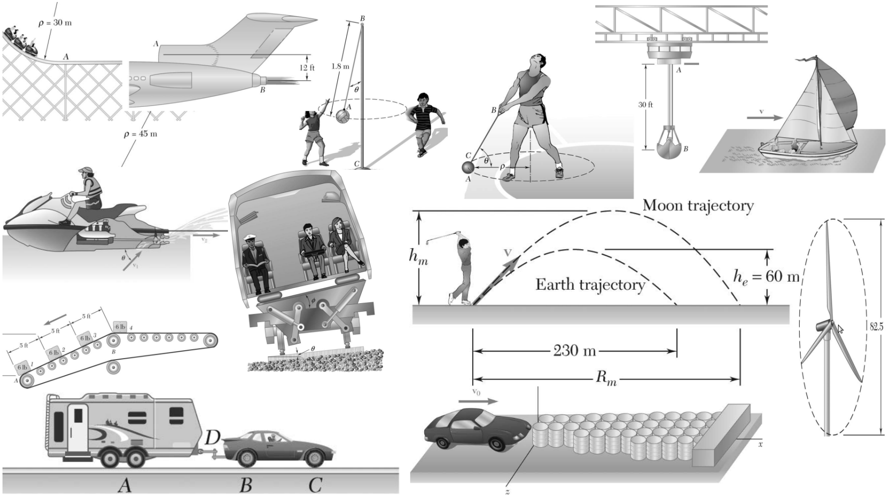
Part 3: Transform domain analysis of linear systems

- 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 systems
- Stability analysis of discrete-time systems

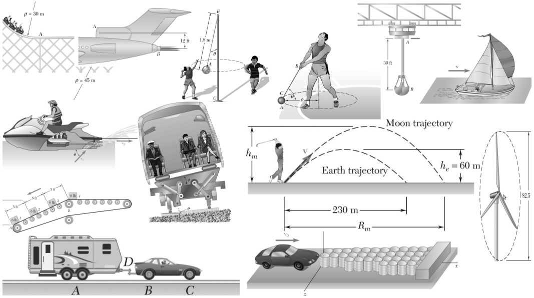
Dynamics?



ρ = 30 m
A
ρ = 45 m
A
B
12 ft
B
1.8 m
θ
A
C
B
C
θ
ρ
A
A
30 ft
B
v
v₂
θ
v₁
Moon trajectory
h_m
v
Earth trajectory
$h_e = 60$ m
82.5
230 m
R_m
5 ft
5 ft
5 ft
6 lb
6 lb
6 lb
6 lb
B
A
φ
θ
D
A
B
C
v₀
x
z

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 may systems relevant to chemical engineering utilise this?

Process dynamics - Change of process variables with time

Transient behaviour during staged-operations

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

i : index for the component

n : index for the plate

h : liquid holdup

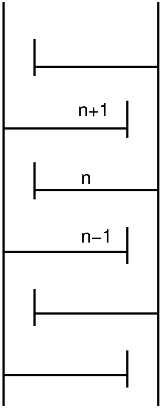
x : mole fraction in the liquid phase

y : mole fraction in the vapour phase

L : liquid flowrate

V : vapour flowrate

Composition in each tray changes with time!!!



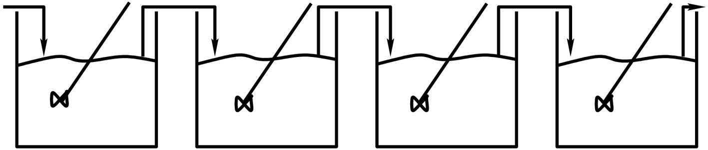
Transient operation of n cascade CSTRs with reversible series reactions

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

$c_1(n)$: concentration of the i^{th} species in the n^{th} reactor

$c_1(0)$: concentration of the i^{th} species in the feed entering the first tank

θ : holding time



Concentrations in the reactors change with time!!!

Transient operation of a jacketed CSTR

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

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

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

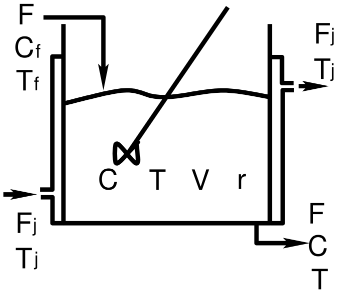
F_j : volumetric flowrate of the heating/cooling fluid

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!!!



Some definitions

Dynamical system

A system is said to be a dynamical system if it has *"at least one"* variable associated with it which is a *"function of time"*.

$$h_n \frac{dx_n(i,t)}{dt} = L_{n-1}x_{n-1}(i,t) + V_{n+1}(t)y_{n+1}(i,t) - V_n(t)y_n(i,t) - L_n(t)x_n(i,t) \quad (5)$$

$$\frac{dc_1(1)}{dt} = -\left(k_1 + \frac{1}{\theta}\right)c_1(1) + k_1' c_2(1) + \frac{1}{\theta}c_1(0) \quad (6)$$

$$\frac{dC}{dt} = \frac{F}{V}(C_f - C) - r \quad (7)$$

$$\frac{dT}{dt} = \frac{F}{V}(T_f - T) + \left(\frac{-\Delta H}{\rho c_p}\right)r - \frac{UA}{V\rho c_p}(T - Tj) \quad (8)$$

Dynamical variable

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

$$h_n \frac{dx_n(i,t)}{dt} = L_{n-1}x_{n-1}(i,t) + V_{n+1}(t)y_{n+1}(i,t) - V_n(t)y_n(i,t) - L_n(t)x_n(i,t) \quad (9)$$

$$\frac{dc_1(1)}{dt} = -\left(k_1 + \frac{1}{\theta}\right)c_1(1) + k_1' c_2(1) + \frac{1}{\theta}c_1(0) \quad (10)$$

$$\frac{dC}{dt} = \frac{F}{V}(C_f - C) - r \quad (11)$$

$$\frac{dT}{dt} = \frac{F}{V}(T_f - T) + \left(\frac{-\Delta H}{\rho c_p}\right)r - \frac{UA}{V\rho c_p}(T - Tj) \quad (12)$$

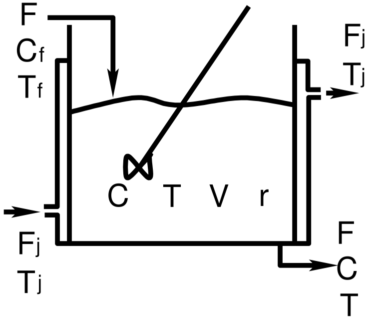
Some definitions

Order of a system - Old definition

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

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

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



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.

Some definitions

Linear system

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

Principle of linearity

If $\hat{L}$ 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 $\hat{L}$ is said to be linear if it satisfies the following:

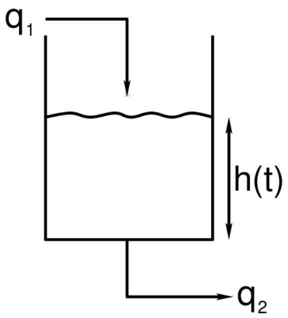
$$\hat{L}(\underline{u} + \underline{v}) = \hat{L}(\underline{u}) + \hat{L}(\underline{v}) \tag{13}$$

$$\hat{L}(\alpha\underline{u}) = \alpha\hat{L}(\underline{u}) \tag{14}$$

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.

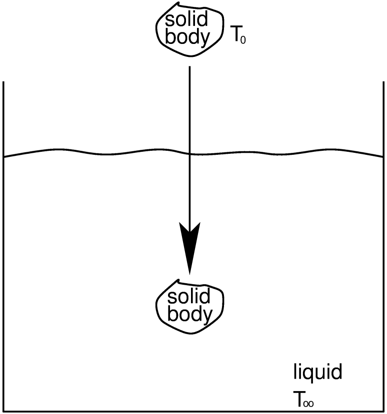
An example of a linear first order system



$$\frac{dh(t)}{dt} = \frac{1}{A}(q_1 - q_2) \tag{15}$$

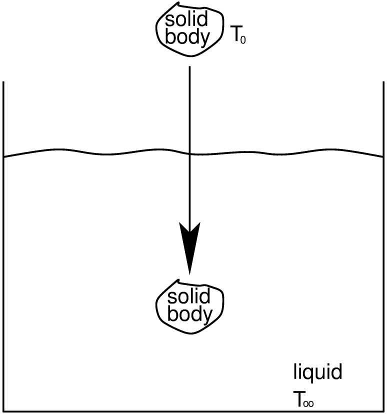
- Dynamical variable: h(t)
- Order of the system = 1

Cooling of a body in an infinite fluid



Consider a liquid reservoir at temperature T_∞ in which a body of temperature T_0 is immersed at time $t = 0$. The time rate of change of temperature of the body as a function of system and material properties can be obtained by modeling the energy balance of the system.

Cooling of a body in an infinite fluid



$$\frac{dT}{dt} = \frac{-hA_s}{\rho Vc}(T - T_\infty) \tag{16}$$

h = heat transfer coefficient

A_s = surface area of the solid body

ρ = density of the solid body

V = volume of the solid body

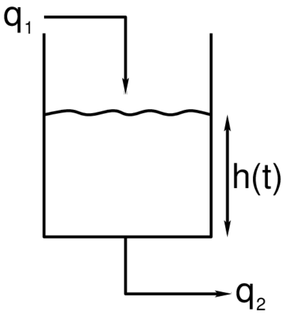
c = specific heat of the solid body

T = instantaneous temperature of the solid body

Cooling of a body in an infinite fluid

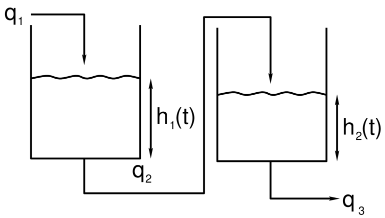
1. What is/are the equilibrium solution(s) of the system?
2. Solve the model equation analytically to determine the time evolution of the system.
3. Develop the phase portrait for the system.
4. Develop the phase portrait without explicitly solving the governing equation.
5. Analyse the solutions and the phase portraits for $T_0 < T_\infty$, $T_0 = T_\infty$ and $T_0 > T_\infty$.
6. Study the effect of different system and material properties on the system dynamics.
7. Comment upon the bifurcation in the system.

Example of a higher order system



$$\frac{dh(t)}{dt} = \frac{1}{A}(q_1 - q_2) \tag{17}$$

- Order of the system $= 1$
- Dynamical variable: $h(t)$



$$\frac{dh_1(t)}{dt} = \frac{1}{A_1}(q_1 - q_2) \tag{18}$$

$$\frac{dh_2(t)}{dt} = \frac{1}{A_2}(q_2 - q_3) \tag{19}$$

- Order of the system $= 2$
- Dynamical variable: $[h_1(t) \;\; h_2(t)]^T$

$$
\begin{aligned}
\frac{dx_1}{dt} &= a_{11}x_1 + a_{12}x_2 + \cdots a_{1N}x_N \\
\frac{dx_2}{dt} &= a_{21}x_1 + a_{22}x_2 + \cdots a_{2N}x_N \\
&\ . \\
&\ . \\
\frac{dx_N}{dt} &= a_{N1}x_1 + a_{N2}x_2 + \cdots a_{NN}x_N
\end{aligned}
$$

- Order of the system $= N$
- Dynamical variable: $[x_1 \quad x_2 \quad \cdots \quad x_N]^T$

Higher order linear autonomous systems

$$\frac{d}{dt}\begin{bmatrix} x_1 \\ x_2 \\ . \\ . \\ x_N \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & . & . & . & a_{1N} \\ a_{21} & a_{22} & . & . & . & a_{2N} \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ a_{N1} & a_{N2} & . & . & . & a_{NN} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ . \\ . \\ . \\ x_N \end{bmatrix} \tag{20}$$

N^{th} order dynamical equation: $\frac{d\underline{x}}{dt} = \underline{\underline{A}}\,\underline{x}$ 1st order dynamical equation: $\frac{dx}{dt} = ax$

Solution of N^{th} order linear autonomous equation

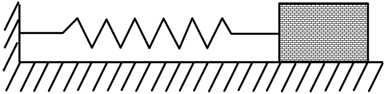
Theorem

The solutions to a linear autonomous equation of the form $\frac{d\underline{x}}{dt} = \underline{\underline{A}}\,\underline{x}$ are given as

$$\underline{x} = \sum_{i=1}^{N} c_i e^{\lambda_i t} \underline{v}_i \quad (21)$$

where,
λ_i's are the eigenvalues of $\underline{\underline{A}}$
$\underline{v}_i$'s are the corresponding eigenvectors
c_i's are present in the field over which the vector space of solutions is defined

Analysis of a free spring-mass system



Consider the case of a single linear spring of spring constant k with mass m attached to it such that the motion of the mass is confined only along the direction of the spring axis. The following equations govern the dynamics of the system.
Free undamped system:

$$m\frac{d^2x}{dt^2} + kx = 0 \tag{22}$$

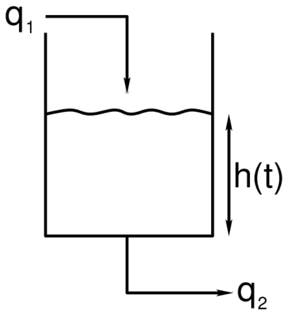
Free vibration with damping:

$$m\frac{d^2x}{dt^2} + c\frac{dx}{dt} + kx = 0 \tag{23}$$

Convert the dynamical equations into matrix equations and analyse

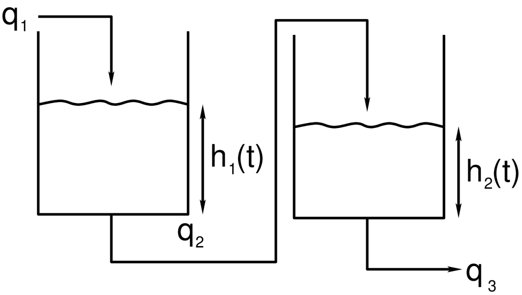
1. the equilibrium solution(s)
2. the phase portraits
3. the stability of the system
4. the effect of different parameters on the dynamical behaviour of the system

Example of a non-autonomous system



$$\frac{dh(t)}{dt} = \frac{1}{A}(q_1 - q_2) \tag{24}$$

Example of a non-autonomous system



$$\frac{dh_1(t)}{dt} = \frac{1}{A_1}(q_1 - q_2) \tag{25}$$

$$\frac{dh_2(t)}{dt} = \frac{1}{A_2}(q_2 - q_3) \tag{26}$$

Transient behaviour during staged-operations

$$h_n \frac{dx_n(i,t)}{dt} = L_{n-1}x_{n-1}(i,t) + V_{n+1}(t)y_{n+1}(i,t) - V_n(t)y_n(i,t) - L_n(t)x_n(i,t) \quad (27)$$

i : index for the component

n : index for the plate

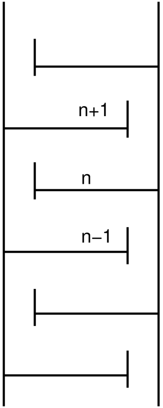
h : liquid holdup

x : mole fraction in the liquid phase

y : mole fraction in the vapour phase

L : liquid flowrate

V : vapour flowrate



A general N^{th} order non-autonomous system

$$\frac{dx_1}{dt} = a_{11}x_1 + a_{12}x_2 + \cdots a_{1N}x_N + b_{11}u_1 + b_{12}u_2 + \cdots b_{1M}u_M$$

$$\frac{dx_2}{dt} = a_{21}x_1 + a_{22}x_2 + \cdots a_{2N}x_N + b_{21}u_1 + b_{22}u_2 + \cdots b_{2M}u_M$$

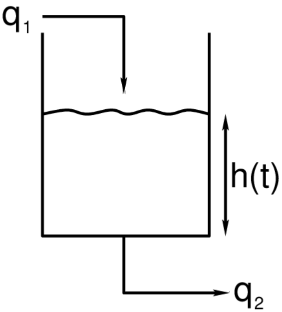
$$\vdots$$

$$\frac{dx_N}{dt} = a_{N1}x_1 + a_{N2}x_2 + \cdots a_{NN}x_N + b_{N1}u_1 + b_{N2}u_2 + \cdots b_{NM}u_M$$

A general N^{th} order non-autonomous system

$$\frac{d}{dt}\begin{bmatrix} x_1 \\ x_2 \\ . \\ . \\ x_N \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & . & . & . & a_{1N} \\ a_{21} & a_{22} & . & . & . & a_{2N} \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ a_{N1} & a_{N2} & . & . & . & a_{NN} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ . \\ . \\ . \\ x_N \end{bmatrix} + \begin{bmatrix} b_{11} & b_{12} & . & . & . & b_{1M} \\ b_{21} & b_{22} & . & . & . & b_{2M} \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ b_{N1} & b_{N2} & . & . & . & b_{NM} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ . \\ . \\ . \\ u_M \end{bmatrix}$$

Output equations



$$\frac{dh(t)}{dt} = \frac{1}{A}(q_1 - q_2) \tag{28}$$

A general N^{th} order non-autonomous system

$$\frac{dx_1}{dt} = a_{11}x_1 + a_{12}x_2 + \cdots a_{1N}x_N + b_{11}u_1 + b_{12}u_2 + \cdots b_{1M}u_M$$

$$\frac{dx_2}{dt} = a_{21}x_1 + a_{22}x_2 + \cdots a_{2N}x_N + b_{21}u_1 + b_{22}u_2 + \cdots b_{2M}u_M$$

$$.$$

$$.$$

$$\frac{dx_N}{dt} = a_{N1}x_1 + a_{N2}x_2 + \cdots a_{NN}x_N + b_{N1}u_1 + b_{N2}u_2 + \cdots b_{NM}u_M$$

$$y_1 = c_{11}x_1 + c_{12}x_2 + \cdots c_{1N}x_N + d_{11}u_1 + d_{12}u_2 + \cdots d_{1M}u_M$$

$$y_2 = c_{21}x_1 + c_{22}x_2 + \cdots c_{2N}x_N + d_{21}u_1 + d_{22}u_2 + \cdots d_{2M}u_M$$

$$.$$

$$.$$

$$y_P = c_{P1}x_1 + c_{P2}x_2 + \cdots c_{PN}x_N + d_{P1}u_1 + d_{P2}u_2 + \cdots d_{PM}u_M$$

A general N^{th} order non-autonomous system

$$\frac{d}{dt}\begin{bmatrix} x_1 \\ x_2 \\ . \\ . \\ x_N \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & . & . & . & a_{1N} \\ a_{21} & a_{22} & . & . & . & a_{2N} \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ a_{N1} & a_{N2} & . & . & . & a_{NN} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ . \\ . \\ . \\ x_N \end{bmatrix} + \begin{bmatrix} b_{11} & b_{12} & . & . & . & b_{1M} \\ b_{21} & b_{22} & . & . & . & b_{2M} \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ b_{N1} & b_{N2} & . & . & . & b_{NM} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ . \\ . \\ . \\ u_M \end{bmatrix}$$

$$\begin{bmatrix} y_1 \\ y_2 \\ . \\ . \\ y_P \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & . & . & . & c_{1N} \\ c_{21} & c_{22} & . & . & . & c_{2N} \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ c_{P1} & c_{P2} & . & . & . & c_{PN} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ . \\ . \\ . \\ x_N \end{bmatrix} + \begin{bmatrix} d_{11} & d_{12} & . & . & . & d_{1M} \\ d_{21} & d_{22} & . & . & . & d_{2M} \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ d_{P1} & d_{P2} & . & . & . & d_{PM} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ . \\ . \\ . \\ u_M \end{bmatrix}$$

A general N^{th} order non-autonomous system

$$\frac{d\underline{x}}{dt} = \underline{\underline{A}}\,\underline{x} + \underline{\underline{B}}\,\underline{u} \tag{29}$$

$$\underline{y} = \underline{\underline{C}}\,\underline{x} + \underline{\underline{D}}\,\underline{u} \tag{30}$$

$\underline{x}$: $N \times 1$

$\underline{y}$: $P \times 1$

$\underline{\underline{A}}$: $N \times N$

$\underline{\underline{B}}$: $N \times M$

$\underline{\underline{C}}$: $P \times N$

$\underline{\underline{D}}$: $P \times M$

Similarity solution: Basic concepts

Similar matrices

If $\underline{\underline{P}}$ is a non-singular matrix such that $\underline{\underline{P}}^{-1}\ \underline{\underline{A}}\ \underline{\underline{P}} = \underline{\underline{B}}$ then $\underline{\underline{A}}$ and $\underline{\underline{B}}$ are called similar matrices.

Similarity transformation

The operation $\underline{\underline{P}}^{-1}\ \underline{\underline{A}}\ \underline{\underline{P}} = \underline{\underline{B}}$ is called similarity transformation.

Important properties of similar matrices

- Similar matrices have same eigenvalues.
- If $\underline{x}$ is an eigenvector of $\underline{\underline{A}}$ with an eigenvalue λ then $\underline{\underline{P}}^{-1}\ \underline{x}$ will be the eigenvector of $\underline{\underline{B}}$ with the same eigenvalue λ.

Similarity solution: Diagonalisation

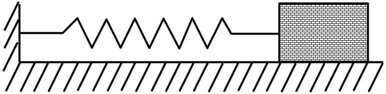
Consider $\underline{\underline{P}}$ made from the augmentation of eigenvectors of $\underline{\underline{A}}$.

$$
\begin{aligned}
\underline{\underline{A}}\ \underline{\underline{P}} &= \underline{\underline{A}}\ [\ \underline{x}_1 \mid \underline{x}_2 \mid \cdots \mid \underline{x}_N\ ] \\
&= [\ \underline{\underline{A}}\ \underline{x}_1 \mid \underline{\underline{A}}\ \underline{x}_2 \mid \cdots \mid \underline{\underline{A}}\ \underline{x}_N\ ] \\
&= [\ \lambda_1\ \underline{x}_1 \mid \lambda_2\ \underline{x}_2 \mid \cdots \mid \lambda_N\ \underline{x}_N\ ] \\
&= \underline{\underline{P}}\ \underline{\underline{\Lambda}}
\end{aligned}
$$

where,

$$
\underline{\underline{\Lambda}} = \begin{bmatrix} \lambda_1 & 0 & . & . & . & 0 \\ 0 & \lambda_2 & . & . & . & 0 \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ 0 & 0 & . & . & . & \lambda_N \end{bmatrix}
$$

Analysis of a forced spring-mass system



Consider the case of a single linear spring of spring constant k with mass m attached to it such that the motion of the mass is confined only along the direction of the spring axis. The following equations govern the dynamics of the system.

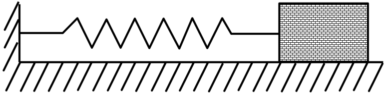
Free undamped system:

$$m\frac{d^2x}{dt^2} + kx = 0 \tag{31}$$

Free vibration with damping:

$$m\frac{d^2x}{dt^2} + c\frac{dx}{dt} + kx = 0 \tag{32}$$

Analysis of a forced spring-mass system



Consider the case of a single linear spring of spring constant k with mass m attached to it such that the motion of the mass is confined only along the direction of the spring axis. The following equations govern the dynamics of the system.

Forced vibration without damping:

$$m\frac{d^2x}{dt^2} + kx = F_0 sin\omega t \tag{33}$$

Forced vibration with damping:

$$m\frac{d^2x}{dt^2} + c\frac{dx}{dt} + kx = F_0 sin\omega t \tag{34}$$

Phase portraits for higher order systems

$$\frac{d}{dt}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \tag{35}$$

$\lambda_1 = a,\ \lambda_2 = b,\ \lambda_3 = c$

$$\underline{v}_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \underline{v}_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \underline{v}_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

Phase portraits for higher order systems

$$\frac{d}{dt}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 & 2 & -1 \\ 0 & 3 & -2 \\ 0 & 2 & -2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \tag{36}$$

$\lambda_1 = 2,\ \lambda_2 = 1,\ \lambda_3 = -1$

$$\underline{v}_1 = \begin{bmatrix} 3 \\ 2 \\ 1 \end{bmatrix}, \underline{v}_2 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \underline{v}_3 = \begin{bmatrix} 0 \\ 1 \\ 2 \end{bmatrix}$$

Phase portraits for higher order systems

$$\frac{d}{dt}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \tag{37}$$

$\lambda_1 = i,\ \lambda_2 = -i,\ \lambda_3 = -1$

$$\underline{v}_1 = \begin{bmatrix} -i \\ 1 \\ 0 \end{bmatrix},\ \underline{v}_2 = \begin{bmatrix} i \\ 1 \\ 0 \end{bmatrix},\ \underline{v}_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

A 4^{th} order linear autonomous system

$$\frac{dx_1}{dt} = x_1 + x_2 - x_3 \tag{38}$$

$$\frac{dx_2}{dt} = x_2 + x_4 \tag{39}$$

$$\frac{dx_3}{dt} = x_3 + x_4 \tag{40}$$

$$\frac{dx_4}{dt} = x_4 \tag{41}$$

A complex reaction system

Consider a system of elementary reaction in series of the type $A \rightarrow B \rightarrow C$. The kinetics of the reaction system is given by the following equations.

$$\frac{dC_A}{dt} = -k_1 C_A \tag{42}$$

$$\frac{dC_B}{dt} = k_1 C_A - k_2 C_B \tag{43}$$

$$\frac{dC_C}{dt} = k_2 C_B \tag{44}$$

The reactions are carried out in a batch reactor with the respective initial concentrations as C_{A0}, C_{B0} and C_{C0}, respectively. Analyse the effects of various parameters associated with the system on the time evolution of the concentrations of the chemical species.

Non-linear systems

Definition: Linear system

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

Principle of linearity

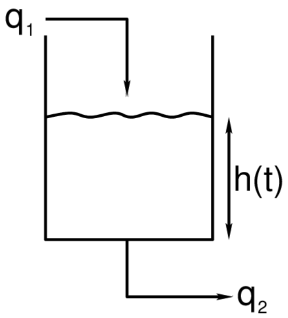
If $\hat{L}$ is an operator in a linear vector space and $\underline{u}$ and $\underline{v}$ are the two vectors in the linear vector space then the operator $\hat{L}$ is said to be linear if it satisfies the following:

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

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

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

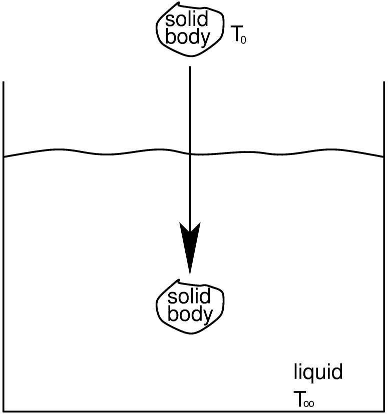
A system not following the above principle of linearity is referred to as a non-linear system.



$$\frac{dh(t)}{dt} = \frac{1}{A}(q_1 - q_2) \tag{45}$$

- Dynamical variable: h(t)
- Order of the system = 1

Non-linear systems



$$\frac{dT}{dt} = \frac{-hA_s}{\rho Vc}(T - T_\infty) \tag{46}$$

h = heat transfer coefficient

A_s = surface area of the solid body

ρ = density of the solid body

V = volume of the solid body

c = specific heat of the solid body

T = instantaneous temperature of the solid body

Linearisation of non-linear systems

$$\frac{d}{dt}\begin{bmatrix} x_1 \\ x_2 \\ . \\ . \\ x_N \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & . & . & . & a_{1N} \\ a_{21} & a_{22} & . & . & . & a_{2N} \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ a_{N1} & a_{N2} & . & . & . & a_{NN} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ . \\ . \\ . \\ x_N \end{bmatrix} + \begin{bmatrix} b_{11} & b_{12} & . & . & . & b_{1M} \\ b_{21} & b_{22} & . & . & . & b_{2M} \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ b_{N1} & b_{N2} & . & . & . & b_{NM} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ . \\ . \\ . \\ u_M \end{bmatrix}$$

$$\begin{bmatrix} y_1 \\ y_2 \\ . \\ . \\ y_P \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & . & . & . & c_{1N} \\ c_{21} & c_{22} & . & . & . & c_{2N} \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ c_{P1} & c_{P2} & . & . & . & c_{PN} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ . \\ . \\ . \\ x_N \end{bmatrix} + \begin{bmatrix} d_{11} & d_{12} & . & . & . & d_{1M} \\ d_{21} & d_{22} & . & . & . & d_{2M} \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ d_{P1} & d_{P2} & . & . & . & d_{PM} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ . \\ . \\ . \\ u_M \end{bmatrix}$$

$$\frac{d\underline{x}}{dt} = \underline{\underline{A}}\,\underline{x} + \underline{\underline{B}}\,\underline{u} \tag{47}$$

$$\underline{y} = \underline{\underline{C}}\,\underline{x} + \underline{\underline{D}}\,\underline{u} \tag{48}$$

$\underline{x}$: $N \times 1$ $\qquad$ $\underline{y}$: $P \times 1$

$\underline{\underline{A}}$: $N \times N$ $\qquad$ $\underline{\underline{B}}$: $N \times M$

$\underline{\underline{C}}$: $P \times N$ $\qquad$ $\underline{\underline{D}}$: $P \times M$

Non-linear dynamical and output equations

$$\frac{dx_1}{dt} = f_1(x_1, x_2, \cdots x_n, u_1, u_2, \cdots u_m)$$

$$\frac{dx_2}{dt} = f_2(x_1, x_2, \cdots x_n, u_1, u_2, \cdots u_m)$$

$$.$$

$$.$$

$$\frac{dx_N}{dt} = f_N(x_1, x_2, \cdots x_n, u_1, u_2, \cdots u_m)$$

$$y_1 = g_1(x_1, x_2, \cdots x_n, u_1, u_2, \cdots u_m)$$

$$y_2 = g_2(x_1, x_2, \cdots x_n, u_1, u_2, \cdots u_m)$$

$$.$$

$$.$$

$$y_P = g_P(x_1, x_2, \cdots x_n, u_1, u_2, \cdots u_m)$$

Linearisation of non-linear systems

Let the steady state of the non-linear system be described by the vector $[x_{1s}\ x_{2s} \cdots x_{ns}\ u_{1s}\ u_{2s} \cdots u_{ms}]^T$

$$
\begin{aligned}
f_i(x_1, x_2, \cdots x_n, u_1, u_2, \cdots u_m) = {} & f_i(x_{1s}, x_{2s}, \cdots x_{ns}, u_{1s}, u_{2s}, \cdots u_{ms}) \\
& + \left.\frac{\partial f_i}{\partial x_1}\right|_{ss} (x_1 - x_{1s}) + \left.\frac{\partial f_i}{\partial x_2}\right|_{ss} (x_2 - x_{2s}) + \cdots \\
& + \left.\frac{\partial f_i}{\partial u_1}\right|_{ss} (u_1 - u_{1s}) + \left.\frac{\partial f_i}{\partial u_2}\right|_{ss} (u_2 - u_{2s}) + \cdots
\end{aligned}
$$

$$
\begin{aligned}
g_j(x_1, x_2, \cdots x_n, u_1, u_2, \cdots u_m) = {} & g_j(x_{1s}, x_{2s}, \cdots x_{ns}, u_{1s}, u_{2s}, \cdots u_{ms}) \\
& + \left.\frac{\partial g_j}{\partial x_1}\right|_{ss} (x_1 - x_{1s}) + \left.\frac{\partial g_j}{\partial x_2}\right|_{ss} (x_2 - x_{2s}) + \cdots \\
& + \left.\frac{\partial g_j}{\partial u_1}\right|_{ss} (u_1 - u_{1s}) + \left.\frac{\partial g_j}{\partial u_2}\right|_{ss} (u_2 - u_{2s}) + \cdots
\end{aligned}
$$

Linearisation of non-linear systems

$$[x_1^* \quad x_2^* \cdots x_N^*] = [(x_1 - x_{1s}) \quad (x_2 - x_{2s}) \cdots (x_N - x_{Ns})]^T$$
$$[u_1^* \quad u_2^* \cdots u_M^*] = [(u_1 - u_{1s}) \quad (u_2 - u_{2s}) \cdots (u_M - u_{Ms})]^T$$
$$[y_1^* \quad y_2^* \cdots y_P^*] = [(y_1 - y_{1s}) \quad (y_2 - y_{2s}) \cdots (y_P - y_{Ps})]^T$$

$$\frac{dx^*}{dt} = \underline{\underline{A}}\ \underline{x}^* + \underline{\underline{B}}\ \underline{u}^* \tag{49}$$

$$y^* = \underline{\underline{C}}\ \underline{x}^* + \underline{\underline{D}}\ \underline{u}^* \tag{50}$$

$$\underline{x}^* = [x_1^* \quad x_2^* \cdots x_N^*]^T; \qquad \underline{u}^* = [u_1^* \quad u_2^* \cdots u_M^*]^T; \qquad \underline{y}^* = [y_1^* \quad y_2^* \cdots y_P^*]^T \tag{51}$$

$$\underline{\underline{A}}_{ij} = \left.\frac{\partial f_i}{\partial x_j}\right|_{ss}; \qquad \underline{\underline{B}}_{ij} = \left.\frac{\partial f_i}{\partial u_j}\right|_{ss}; \qquad \underline{\underline{C}}_{ij} = \left.\frac{\partial g_i}{\partial x_j}\right|_{ss}; \qquad \underline{\underline{D}}_{ij} = \left.\frac{\partial g_i}{\partial x_j}\right|_{ss} \tag{52}$$

Linear *vs.* non-linear population growth models

A linear model for population growth:
Assumptions

- Population confined to the region *i.e.* no entry and exit of members
- Growth rate is a function of the instantaneous population
- No *death*; *birth* only from the present members, no explicit birth rate term

Linear *vs.* non-linear population growth models

A non-linear model for population growth:
Assumptions to overcome the issues of the linear model

- Population confined to the region *i.e.* no entry and exit of members
- Growth rate is a function of the instantaneous population
- No *death*; *birth* only from the present members, no explicit birth rate term
- Growth rate proportional to the instantaneous population only for small populations
- Negative growth rate at large populations so as to "limit" the population

$$\frac{dx}{dt} = ax\left(1 - \frac{x}{N}\right) \tag{53}$$

Logistic population growth model with harvesting

A non-linear model for population growth:
Assumptions to overcome the issues of the linear model

- Population confined to the region *i.e.* no entry but exit of members at a constant rate
- Growth rate is a function of the instantaneous population
- No *death*; *birth* only from the present members, no explicit birth rate term
- Growth rate proportional to the instantaneous population only for small populations
- Negative growth rate at large populations so as to "limit" the population

$$\frac{dx}{dt} = ax\left(1 - \frac{x}{N}\right) - h \tag{54}$$

Logistic population growth with critical threshold

The logistic growth model for the population growth of a species accounted for *carrying capacity* of the system. Imagine a population which goes to extinction if the initial population if below a certain number *i.e.* there exists a *threshold population* for the species to survive. The features of such a population dynamics are:

- Upper limit on the population based on the carrying capacity
- Exponential growth at initial stages and saturation at later stages
- Extinction when the initial population is less than the threshold population

$$\frac{dx}{dt} = -ax\left(1 - \frac{x}{\lambda_1}\right)\left(1 - \frac{x}{\lambda_2}\right) \tag{55}$$

λ_1: carrying capacity; λ_2: threshold population; $0 < \lambda_2 < \lambda_1$

Bifurcations in non-linear systems

$$\frac{dx}{dt} = ax - ax^2 \tag{56}$$

$$\frac{dx}{dt} = a - x^2 \tag{57}$$

$$\frac{dx}{dt} = ax - x^2 \tag{58}$$

$$\frac{dx}{dt} = ax - x^3 \tag{59}$$

$$\frac{dx_1}{dt} = -x_1 \tag{60}$$

$$\frac{dx_2}{dt} = x_1^2 + x_2 \tag{61}$$

Non-linear systems in higher dimensions

$$\frac{dx_1}{dt} = x_1^2 \tag{62}$$

$$\frac{dx_2}{dt} = -x_2 \tag{63}$$

Non-linear systems in higher dimensions

Hartman-Grobman theorem

The orbit structure of a dynamical system in the neighbourhood of a hyperbolic equilibrium point is topologically equivalent to the orbit structure of its linearised system

Non-linear systems in higher dimensions

$$\frac{dx_1}{dt} = x_1^2 - x_2^2 - 1 \quad (64)$$

$$\frac{dx_2}{dt} = 2x_2 \quad (65)$$

Transient operation of a jacketed CSTR

$$\frac{dC}{dt} = \frac{F}{V}(C_f - C) - r \tag{66}$$

$$\frac{dT}{dt} = \frac{F}{V}(T_f - T) + \left(\frac{-\Delta H}{\rho c_p}\right) r - \frac{UA}{V\rho c_p}(T - T_j) \tag{67}$$

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