CHE302 LECTURE IV
MATHEMATICAL MODELING OF CHEMICAL PROCESS

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THE RATIONALE FOR MATHEMATICAL MODELING

- ## Where to use

  - To improve understanding of the process
  - To train plant operating personnel
  - To design the control strategy for a new process
  - To select the controller setting
  - To design the control law
  - To optimize process operating conditions

- ## A Classification of Models

  - Theoretical models (based on physicochemical law)
  - Empirical models (based on process data analysis)
  - Semi-empirical models (combined approach)

DYNAMIC VERSUS STEADY-STATE MODEL

- ## Dynamic model
  - **Describes time behavior of a process**
    - **Changes in input, disturbance, parameters, initial condition, etc.**
  - **Described by a set of differential equations**
    : ordinary (ODE), partial (PDE), differential-algebraic(DAE)

  Initial Condition, x(0)

  Input, u(t)   **Output, y(t)**

  Dynamic Model
  (ODE, PDE)

  Parameter, p(t)
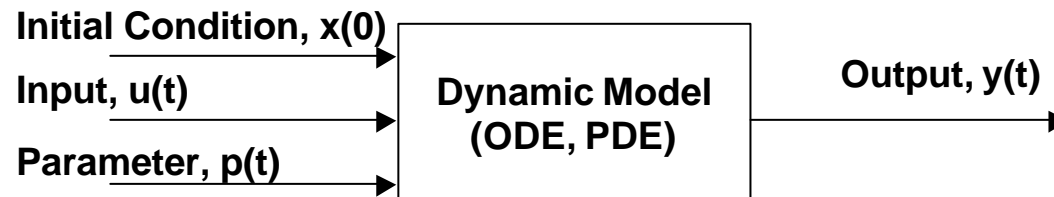
- ## Steady-state model
  - **Steady state: No further changes in all variables**
  - **No dependency in time: No transient behavior**
  - **Can be obtained by setting the time derivative term zero**

MODELING PRINCIPLES

- ## Conservation law
  - **Within a defined system boundary (control volume)**

$$\begin{bmatrix} \text{rate of} \\ \text{accumulation} \end{bmatrix} = \begin{bmatrix} \text{rate of} \\ \text{input} \end{bmatrix} - \begin{bmatrix} \text{rate of} \\ \text{output} \end{bmatrix}$$

$$+ \begin{bmatrix} \text{rate of} \\ \text{generation} \end{bmatrix} - \begin{bmatrix} \text{rate of} \\ \text{disappreance} \end{bmatrix}$$

- ## Mass balance (overall, components)

- ## Energy balance

- ## Momentum or force balance

- ## Algebraic equations: relationships between variables and parameters

MODELING APPROACHES

- **Theoretical Model**
  - Follow conservation laws
  - Based on physicochemical laws
  - Variables and parameters have physical meaning
  - Difficult to develop
  - Can become quite complex
  - Extrapolation is valid unless the physicochemical laws are invalid
  - Used for optimization and rigorous prediction of the process behavior

- **Empirical model**
  - Based on the operation data
  - Parameters may not have physical meaning
  - Easy to develop
  - Usually quite simple
  - Requires well designed experimental data
  - The behavior is correct only around the experimental condition
  - Extrapolation is usually invalid
  - Used for control design and simplified prediction model

DEGREE OF FREEDOM (DOF) ANALYSIS

- **DOF**
  - **Number of variables that can be specified independently**
  - $N_F = N_V - N_E$
    - N_F : **Degree of freedom (no. of independent variables)**
    - N_V : **Number of variables**
    - N_E : **Number of equations (no. of dependent variables)**
    - **Assume no equation can be obtained by a combination of other equations**

- **Solution depending on DOF**
  - **If $N_F = 0$, the system is *exactly determined*. Unique solution exists.**
  - **If $N_F > 0$, the system is *underdetermined*. Infinitely many solutions exist.**
  - **If $N_F < 0$, the system is *overdetermined*. No solutions exist.**

LINEAR VERSUS NONLINEAR MODELS

- **Superposition principle**

  $\forall \boldsymbol{a}, \boldsymbol{b} \in \Re,$ and for a linear operator, L

  Then $L(\boldsymbol{a}\, x_1(t) + \boldsymbol{b}\, x_2(t)) = \boldsymbol{a}\, L(x_1(t)) + \boldsymbol{b}\, L(x_2(t))$

- **Linear dynamic model: superposition principle holds**

  $\forall \boldsymbol{a}, \boldsymbol{b} \in \Re,\; u_1(t) \rightarrow y_1(t)$ and $u_2(t) \rightarrow y_2(t)$

  $\boldsymbol{a}\, u_1(t) + \boldsymbol{b}\, u_2(t) \rightarrow \boldsymbol{a}\, y_1(t) + \boldsymbol{b}\, y_2(t)$

  $\forall \boldsymbol{a}, \boldsymbol{b} \in \Re,\; x_1(0) \rightarrow y_1(t)$ and $x_2(0) \rightarrow y_2(t)$

  $\boldsymbol{a}\, x_1(0) + \boldsymbol{b}\, x_2(0) \rightarrow \boldsymbol{a}\, y_1(t) + \boldsymbol{b}\, y_2(t)$

  - **Easy to solve and analytical solution exists.**
  - **Usually, locally valid around the operating condition**

- **Nonlinear: "Not linear"**

  - **Usually, hard to solve and analytical solution does not exist.**

ILLUSTRATION OF SUPERPOSITION PRINCIPLE
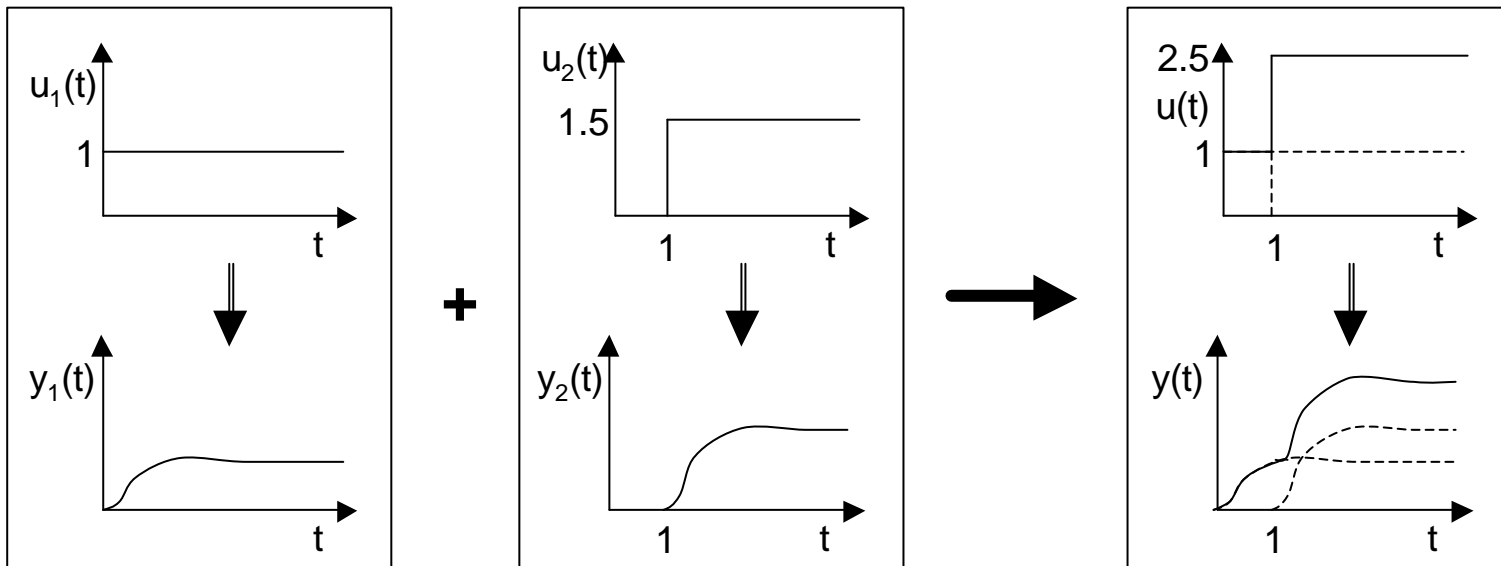
- ## Valid only for linear process
  - For example, if $y(t)=u(t)^2$,

    $(u_1(t)+1.5u_2(t))^2$ is not same as $u_1(t)^2 +1.5u_2(t)^2$.

TYPICAL LINEAR DYNAMIC MODEL

- **Linear ODE**

$$t\frac{dy(t)}{dt} = -y(t) + Ku(t) \quad (t \text{ and K are contant, 1st order})$$

$$\frac{d^n y(t)}{dt^n} + a_{n-1}\frac{d^{n-1}y(t)}{dt^{n-1}} + \ldots + a_0 y(t)$$

$$= b_m\frac{d^m u(t)}{dt^m} + b_{m-1}\frac{d^{m-1}u(t)}{dt^{m-1}} + \ldots + b_0 u(t) \quad (\text{nth order})$$

- **Nonlinear ODE**

$$t\frac{dy(t)}{dt} = -y(t)^2 + Ku(t) \qquad t\frac{dy(t)}{dt}y(t) = -y(t)\sin(y) + Ku(t)$$
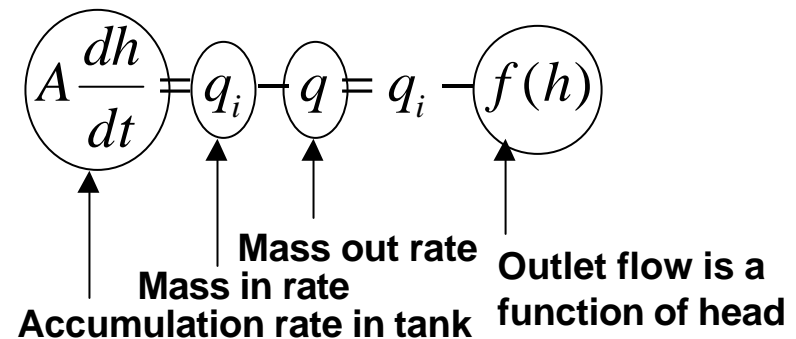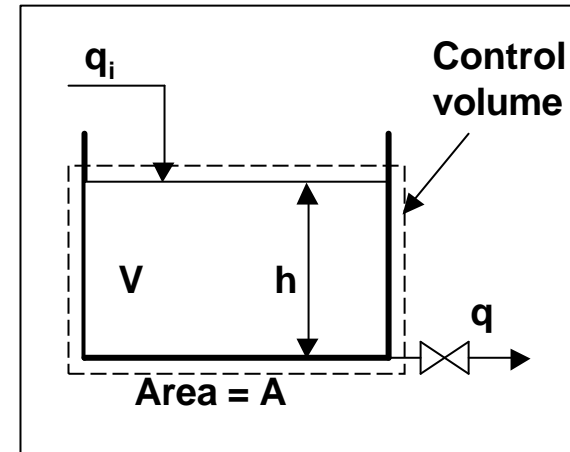
$$t\frac{dy(t)}{dt} = -y(t) + K\sqrt{u(t)} \qquad t\frac{dy(t)}{dt} = -e^{-y(t)} + Ku(t)$$

MODELS OF REPRESENTATIVE PROCESSES

- **Liquid storage systems**

  - System boundary: storage tank
  - Mass in: q_i (vol. flow, indep. var)
  - Mass out: q (vol, flow, dep. var)
  - No generation or disappearance (no reaction or leakage)
  - No energy balance

  - DOF=2 (h, q_i) - 1=1
  - If $f(h) = h/R_V$, the ODE is linear. (R_V is the resistance to flow)
  - If $f(h) = C_V \sqrt{rgh/g_c}$, the ODE is nonlinear. (C_V is the valve constant)

$$A\frac{dh}{dt} = q_i - q = q_i - f(h)$$

Mass out rate
Mass in rate
Accumulation rate in tank
Outlet flow is a function of head

- **Continuous Stirred Tank Reactor (CSTR)**
  - **Liquid level is constant** (No acc. in tank)
  - **Constant density, perfect mixing**
  - **Reaction: A → B** ($r = k_0 \exp(-E/RT)c_A$)
  - **System boundary: CSTR tank**
 - **Component mass balance**

$$V \frac{dc_A}{dt} = q(c_{Ai} - c_A) - Vkc_A$$

  - **Energy balance**

$$V r C_p \frac{dT}{dt} = q r C_p (T_i - T) + (-\Delta H)Vkc_A + UA(T_c - T)$$

  - **DOF analysis**
    - **No. of variables: 6** (q, c_A, c_{Ai}, T_i, T, T_c)
    - **No. of equation:2 (two dependent vars.:** c_A, T)
    - **DOF=6 – 2 = 4**
    - **Independent variables: 4** (q, c_{Ai}, T_i, T_c)
    - **Parameters: kinetic parameters,** V, U, A, **other physical properties**
    - **Disturbances: any of** q, c_{Ai}, T_i, T_c, **which are not manipulatable**

c_{Ai}, q_i, T_i

c_A, q, T

V, T   h

Cooling
medium, T_c
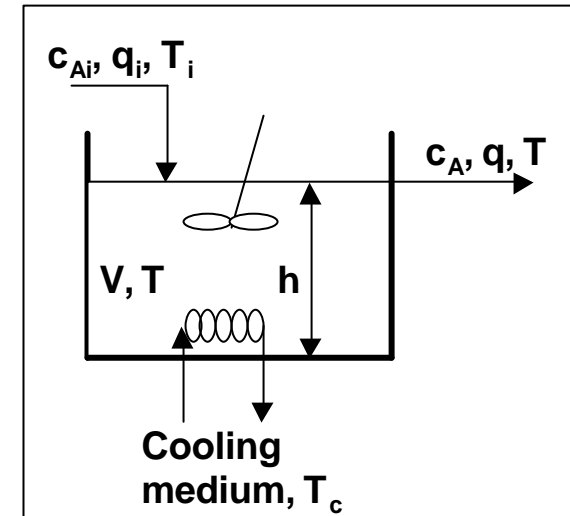
STANDARD FORM OF MODELS

From the previous example

$$\frac{dc_A}{dt} = \frac{q}{V}(c_{Ai} - c_A) - kc_A = f_1(c_A, T, q, c_{Ai})$$

$$\frac{dT}{dt} = \frac{q}{V}(T_i - T) + \frac{q}{rC_p}(-\Delta H)kc_A + \frac{UA}{rC_p}(T_c - T) = f_2(c_A, T, q, T_c, T_i)$$

- **State-space model**

  $$\dot{\mathbf{x}} = d\mathbf{x}/dt = \mathbf{f}(\mathbf{x}, \mathbf{u}, \mathbf{d})$$

  where $\mathbf{x} = [x_1, \cdots, x_n]^T, \mathbf{u} = [u_1, \cdots, u_m]^T, \mathbf{d} = [d_1, \cdots, d_l]^T$

  - **x: states, $[c_A \ T]^T$**
  - **u: inputs, $[q \ T_c]^T$**
  - **d: disturbances, $[c_{Ai} \ T_i]^T$**
  - **y: outputs – can be a function of above, y=g(x,d,u), $[c_A \ T]^T$**
  - **If higher order derivatives exist, convert them to 1st order.**

CONVERT TO 1$^{\text{ST}}$-ORDER ODE

- **Higher order ODE**

$$\frac{d^n x(t)}{dt^n} + a_{n-1}\frac{d^{n-1}x(t)}{dt^{n-1}} + \ldots + a_0 x(t) = b_0 u(t)$$

- **Define new states**

$$x_1 = x, \ x_2 = \dot{x}, \ x_3 = \ddot{x}, \ \cdots, \ x_n = x^{(n-1)}$$

- **A set of 1$^{\text{st}}$-order ODE's**

$$\dot{x}_1 = x_2$$

$$\dot{x}_2 = x_3$$

$$\vdots$$

$$\dot{x}_n = -a_{n-1}x_n - a_{n-2}x_{n-1} - \cdots - a_0 x_1 + b_0 u$$

SOLUTION OF MODELS

- ## ODE (state-space model)

  - Linear case: find the analytical solution via Laplace transform, or other methods.

  - Nonlinear case: analytical solution usually does not exist.

    - Use a numerical integration, such as *RK method*, by defining initial condition, time behavior of input/disturbance

    - Linearize around the operating condition and find the analytical solution

- ## PDE

  - Convert to ODE by discretization of spatial variables using *finite difference approximation* and etc.

$$\frac{\partial T_L}{\partial t} = -v\frac{\partial T_L}{\partial z} + \frac{1}{t_{HL}}(T_w - T_L) \quad \longrightarrow \quad \frac{dT_L(j)}{dt} = -\frac{v}{\Delta z}T_L(j-1) - \left(\frac{v}{\Delta z} + \frac{1}{t_{HL}}\right)T_L(j) + \frac{1}{t_{HL}}T_w$$

$$\frac{\partial T_L}{\partial z} \approx \frac{T_L(j) - T_L(j-1)}{\Delta z} \qquad\qquad (j = 1, \cdots N)$$

LINEARIZATION

- ## Equilibrium (Steady state)
  - Set the derivatives as zero: $0 = \mathbf{f}(\overline{\mathbf{x}}, \overline{\mathbf{u}}, \overline{\mathbf{d}})$
  - Overbar denotes the steady-state value and $(\overline{\mathbf{x}}, \overline{\mathbf{u}}, \overline{\mathbf{d}})$ is the equilibrium point. (could be multiple)
  - Solve them analytically or numerically using *Newton method*

- ## Linearization around equilibrium point
  - Taylor series expansion to 1st order

$$\mathbf{f}(\mathbf{x}, \mathbf{u}) = \mathbf{f}(\overline{\mathbf{x}}, \overline{\mathbf{u}})^{\nearrow 0} + \left.\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right|_{(\overline{\mathbf{x}}, \overline{\mathbf{u}})} (\mathbf{x} - \overline{\mathbf{x}}) + \left.\frac{\partial \mathbf{f}}{\partial \mathbf{u}}\right|_{(\overline{\mathbf{x}}, \overline{\mathbf{u}})} (\mathbf{u} - \overline{\mathbf{u}}) + \cdots$$

Jacobian

$$\frac{\partial \mathbf{f}}{\partial \mathbf{x}} = \begin{bmatrix} \dfrac{\partial f_1}{\partial x_1} & \cdots & \dfrac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \dfrac{\partial f_n}{\partial x_1} & \cdots & \dfrac{\partial f_n}{\partial x_n} \end{bmatrix}$$

  - Ignore higher order terms
  - Define deviation variables: $\mathbf{x}' = \mathbf{x} - \overline{\mathbf{x}}, \quad \mathbf{u}' = \mathbf{u} - \overline{\mathbf{u}}$

$$\dot{\mathbf{x}}' = \left.\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right|_{(\overline{\mathbf{x}}, \overline{\mathbf{u}})} \mathbf{x}' + \left.\frac{\partial \mathbf{f}}{\partial \mathbf{u}}\right|_{(\overline{\mathbf{x}}, \overline{\mathbf{u}})} \mathbf{u}' = \mathbf{A}\mathbf{x}' + \mathbf{B}\mathbf{u}'$$