CHE302 LECTURE IV
MATHEMATICAL MODELING OF CHEMICAL PROCESS

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Fall 2001

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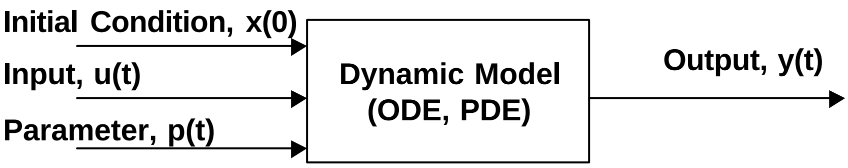
THE RATIONALE FOR MATHEMATICAL MODELING

- **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)



- **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**

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

  Then $L(a\,x_1(t) + b\,x_2(t)) = a\,L(x_1(t)) + b\,L(x_2(t))$
- **Linear dynamic model: superposition principle holds**

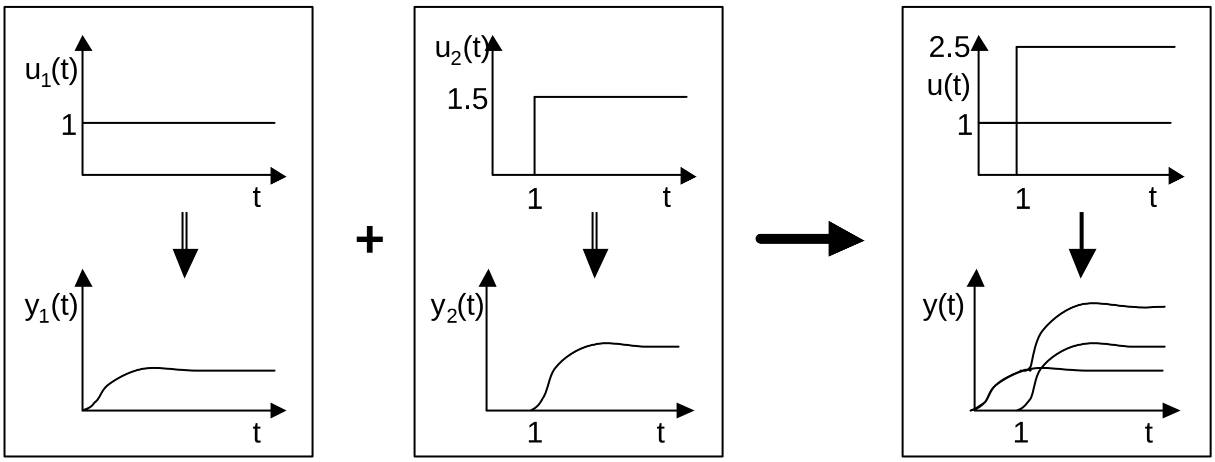
  $$\forall a, b \in \Re,\ u_1(t) \rightarrow y_1(t) \text{ and } u_2(t) \rightarrow y_2(t)$$
  $$a\,u_1(t) + b\,u_2(t) \rightarrow a\,y_1(t) + b\,y_2(t)$$
  $$\forall a, b \in \Re,\ x_1(0) \rightarrow y_1(t) \text{ and } x_2(0) \rightarrow y_2(t)$$
  $$a\,x_1(0) + b\,x_2(0) \rightarrow a\,y_1(t) + b\,y_2(t)$$

  – **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**

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

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

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

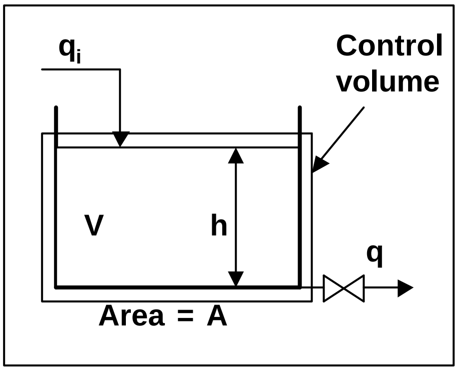
- **Nonlinear ODE**

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

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

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**

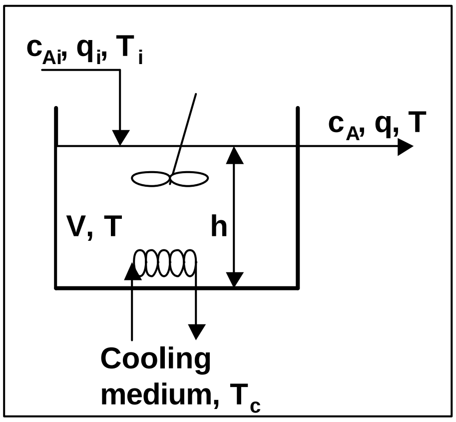


$$A\frac{dh}{dt} = q_i - q = q_i - f(h)$$

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

  - **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)**

- **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**

STANDARD FORM OF MODELS

From the previous example

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

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

- **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 1ST-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 1st-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.**

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

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

LINEARIZATION

- **Equilibrium (Steady state)**
  - **Set the derivatives as zero:** $\mathbf{0} = \mathbf{f}(\bar{\mathbf{x}}, \bar{\mathbf{u}}, \bar{\mathbf{d}})$
  - **Overbar denotes the steady-state value and** $(\bar{\mathbf{x}}, \bar{\mathbf{u}}, \bar{\mathbf{d}})$ **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**

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

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

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

Jacobian

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