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)

![Dynamic Model Diagram](image)

- Initial Condition, \(x(0)\)
- Input, \(u(t)\)
- Parameter, \(p(t)\)
- Dynamic Model (ODE, PDE)
- Output, \(y(t)\)

• **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)
  \[
  \begin{bmatrix}
  \text{rate of accumulation} \\
  \end{bmatrix} = \begin{bmatrix}
  \text{rate of input} \\
  \end{bmatrix} - \begin{bmatrix}
  \text{rate of output} \\
  \end{bmatrix} \\
  + \begin{bmatrix}
  \text{rate of generation} \\
  \end{bmatrix} - \begin{bmatrix}
  \text{rate of disappearance} \\
  \end{bmatrix}
  \]

• 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

\[ \forall \alpha, \beta \in \mathbb{R}, \text{ and for a linear operator, } L \]

Then \[ L(\alpha x_1(t) + \beta x_2(t)) = \alpha L(x_1(t)) + \beta L(x_2(t)) \]

• Linear dynamic model: superposition principle holds

\[ \forall \alpha, \beta \in \mathbb{R}, \ u_1(t) \rightarrow y_1(t) \text{ and } u_2(t) \rightarrow y_2(t) \]

\[ \alpha u_1(t) + \beta u_2(t) \rightarrow \alpha y_1(t) + \beta y_2(t) \]

\[ \forall \alpha, \beta \in \mathbb{R}, \ x_1(0) \rightarrow y_1(t) \text{ and } x_2(0) \rightarrow y_2(t) \]

\[ \alpha x_1(0) + \beta x_2(0) \rightarrow \alpha y_1(t) + \beta y_2(t) \]

– 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**

\[
\tau \frac{dy(t)}{dt} = -y(t) + Ku(t) \quad (\tau \text{ and } K \text{ are constant, 1st order})
\]

\[
\frac{d^n y(t)}{dt^n} + a_{n-1} \frac{d^{n-1} y(t)}{dt^{n-1}} + \ldots + a_0 y(t) = b_m \frac{d^m u(t)}{dt^m} + b_{m-1} \frac{d^{m-1} u(t)}{dt^{m-1}} + \ldots + b_0 u(t) \quad (\text{nth order})
\]

• **Nonlinear ODE**

\[
\tau \frac{dy(t)}{dt} = -y(t)^2 + Ku(t)
\]

\[
\tau \frac{dy(t)}{dt} = -y(t)\sin(y) + Ku(t)
\]

\[
\tau \frac{dy(t)}{dt} = -y(t) + K\sqrt{u(t)}
\]

\[
\tau \frac{dy(t)}{dt} = -e^{-y(t)} + Ku(t)
\]
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.
    \((R_V \text{ is the resistance to flow})\)
  – If \(f(h) = C_V \sqrt{\rho gh / g_c}\), the ODE is nonlinear.
    \((C_V \text{ is the valve constant})\)

\[
A \frac{dh}{dt} = q_i - q - f(h)
\]
• Continuous Stirred Tank Reactor (CSTR)
  – Liquid level is constant (No acc. in tank)
  – Constant density, perfect mixing
  – Reaction: \( A \rightarrow B \) \( (r = k_0 e^{-E/RT}c_A) \)
  – System boundary: CSTR tank
  – Component mass balance
    \[
    V \frac{dc_A}{dt} = q(c_{Ai} - c_A) - Vkc_A
    \]
  – Energy balance
    \[
    V \rho C_p \frac{dT}{dt} = q \rho C_p (T_i - T) + (\Delta H)Vkc_A + UA(T_c - T)
    \]
  – 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

\[
\frac{d c_A}{dt} = \frac{q}{V} (c_{Ai} - c_A) - k c_A = f_1(c_A, T, q, c_{Ai})
\]

\[
\frac{d T}{dt} = \frac{q}{V} (T_i - T) + \frac{q}{\rho C_p} (-\Delta H) k c_A + \frac{UA}{\rho C_p} (T_c - T) = f_2(c_A, T, q, T_c, T_i)
\]

- **State-space model**
  \[
  \dot{x} = \frac{dx}{dt} = f(x, u, d)
  \]
  where \(x = [x_1, \cdots, x_n]^T, u = [u_1, \cdots, u_m]^T, d = [d_1, \cdots, d_l]^T\)
  - \(x\): 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 1\(^{st}\) order.
CONVERT TO 1\textsuperscript{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

\[
x_1 = x, \quad x_2 = \dot{x}, \quad x_3 = \ddot{x}, \quad \ldots, \quad x_n = x^{(n-1)}
\]

- A set of 1\textsuperscript{st}-order ODE’s

\[
\begin{align*}
\dot{x}_1 &= x_2 \\
\dot{x}_2 &= x_3 \\
& \vdots \\
\dot{x}_n &= -a_{n-1}x_n - a_{n-2}x_{n-1} - \ldots - a_0 x_1 + b_0 u
\end{align*}
\]
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.

\[
\frac{dT_L}{dt} = -\nu \frac{\partial T_L}{\partial z} + \frac{1}{\tau_{HL}} (T_w - T_L)
\]

\[
\frac{dT_L(j)}{dt} = -\frac{\nu}{\Delta z} T_L(j-1) - \left( \frac{\nu}{\Delta z} + \frac{1}{\tau_{HL}} \right) T_L(j) + \frac{1}{\tau_{HL}} T_w
\]

\[
\frac{\partial T_L}{\partial z} \approx \frac{T_L(j) - T_L(j-1)}{\Delta z}
\]

\[
(j = 1, \ldots, N)
\]
LINEARIZATION

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

• **Linearization around equilibrium point**
  
  – Taylor series expansion to \(1^{\text{st}}\) order
    \[
    f(x, u) = f(\bar{x}, \bar{u}) + \left. \frac{\partial f}{\partial x} \right|_{(\bar{x}, \bar{u})} (x - \bar{x}) + \left. \frac{\partial f}{\partial u} \right|_{(\bar{x}, \bar{u})} (u - \bar{u}) + \cdots
    \]
  
  – Ignore higher order terms
  
  – Define deviation variables: \( x' = x - \bar{x}, \ u' = u - \bar{u} \)
  
  \[
  \dot{x}' = \left. \frac{\partial f}{\partial x} \right|_{(\bar{x}, \bar{u})} x' + \left. \frac{\partial f}{\partial u} \right|_{(\bar{x}, \bar{u})} u' = Ax' + Bu'
  \]

\[\text{Jacobian} = \begin{bmatrix}
    \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\
    \vdots & \ddots & \vdots \\
    \frac{\partial f_n}{\partial x_1} & \cdots & \frac{\partial f_n}{\partial x_n}
\end{bmatrix}\]