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, \( u(t) \)
  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 to zero

MODELING PRINCIPLES

• Conservation law
  – Within a defined system boundary (control volume)
    \[
    \begin{bmatrix}
    \text{rate of accumulation} \\
    \text{output} \\
    \text{disappearance}
    \end{bmatrix}
    = \begin{bmatrix}
    \text{rate of input} \\
    \text{rate of generation}
    \end{bmatrix}
    \]

• 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

LINEAR VERSUS NONLINEAR MODELS

- **Superposition principle**
  \( \forall \alpha, \beta \in \mathbb{R}, \) and for a linear operator, \( L \)
  \[ L(\alpha x_1(t) + \beta x_2(t)) = \alpha L(x_1(t)) + \beta L(x_2(t)) \]

- **Linear dynamic model: superposition principle holds**
  \( \forall \alpha, \beta \in \mathbb{R}, \) \( u_1(t) \rightarrow y_1(t) \) and \( u_2(t) \rightarrow y_2(t) \)
  \[ \alpha u_1(t) + \beta u_2(t) \rightarrow \alpha y_1(t) + \beta y_2(t) \]

- **Nonlinear: “Not linear”**
  - Usually, hard to solve and analytical solution does not exist.

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.

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
  \[ \tau \frac{dy(t)}{dt} = -y(t) + Ku(t) \quad (\tau \text{ and } K \text{ are contant, 1st order}) \]
  \[ \frac{d^n y(t)}{dt^n} + a_{n-1} \frac{d^{n-1} y(t)}{dt^{n-1}} + \ldots + a_0 y(t) = b_n \frac{d^n u(t)}{dt^n} + b_{n-1} \frac{d^{n-1} u(t)}{dt^{n-1}} + \ldots + b_0 u(t) \quad (\text{nth order}) \]

- Nonlinear ODE
  \[ \tau \frac{dy(t)}{dt} = -y(t)^2 + Ku(t) \quad \tau \frac{dy(t)}{dt} = -y(t) \sin(y) + Ku(t) \]
  \[ \tau \frac{dy(t)}{dt} = -y(t) + K u(t) \quad \tau \frac{dy(t)}{dt} = e^{-y(t)} + Ku(t) \]

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 \( f(h) = h/R \), the ODE is linear. \((R_V = \text{the resistance to flow})\)
  - If \( f(h) = C_i \sqrt{ghh} \), the ODE is nonlinear. \((C_V = \text{the valve constant})\)

STANDARD FORM OF MODELS

- Continuous Stirred Tank Reactor (CSTR)
  - Liquid level is constant \((\text{No acc. in tank})\)
  - Constant density, perfect mixing
  - Reaction: \( A \rightarrow B \quad (r = k_\text{exp}(E/RT)c_A) \)
  - System boundary: CSTR tank
  - Component mass balance
    \[ V \frac{dc_A}{dt} = q(c_A - c_A) - V k c_A \]
  - Energy balance
    \[ \frac{dT}{dt} = \frac{q}{V}(T_i - T) + \frac{q}{C_P}(-\Delta H)k c_A + \frac{UA}{C_P}(T_c - T) \]
  - DOF analysis
    - No. of variables: 6 \((q, c_A, c_A, T_i, T_c)\)
    - No. of equation: 2 \((\text{two dependent vars.}: c_A, T_i)\)
    - DOF=6-2=4
    - Independent variables: 4 \((q, c_A, T_i, T_c)\)
    - Parameters: kinetic parameters, \( V, U, A \) and other physical properties
    - Disturbances: any of \( q, c_A, T_i, T_c \) which are not manipulatable

From the previous example

\[ \frac{dc_A}{dt} = \frac{q}{V}(c_A - c_A) - k c_A = f_1(c_A, T, q, c_A) \]
\[ \frac{dT}{dt} = \frac{q}{V}(T_i - T) + \frac{q}{p C_P}(-\Delta H)k c_A + \frac{UA}{p C_P}(T_c - T) = f_2(c_A, T, q, T, T_c) \]

- State-spacemodel
  \[ x = dx/dt = f(x, u, d) \]
  where \( x = [x_1, \ldots, x_n]^T, u = [u_1, \ldots, u_m]^T, d = [d_1, \ldots, d_l]^T \)
  - \( x \): states, \([c_A, T]^T\)
  - \( u \): inputs, \([q, T_i]^T\)
  - \( d \): disturbances, \([c_A, T_i]^T\)
  - \( y \): 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
  \[ x_1 = x, \; x_2 = \dot{x}, \; x_3 = \ddot{x}, \; \ldots, \; x_n = x^{(n-1)} \]

- A set of 1st-order ODE's

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

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 1st order
  \[ f(x, u) = f(\bar{x}, \bar{u}) + \frac{\partial f}{\partial x}(x - \bar{x}) + \frac{\partial f}{\partial u}(u - \bar{u}) + \ldots \]
  - Ignore higher order terms
  - Define deviation variables: \( x' = x - \bar{x}, \; u' = u - \bar{u} \)

\[ \begin{bmatrix} \dot{x}_1 \\ \vdots \\ \dot{x}_n \end{bmatrix} = A \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} + B u' \]

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.

\[ \begin{align*}
  \frac{\partial T_j}{\partial t} &= -v \frac{\partial T_j}{\partial z} + \frac{1}{\tau_M} (T_j - T_i) \\
  \frac{\partial T_i}{\partial z} &= \frac{T_i(j) - T_i(j-1)}{\Delta z} \\
  \frac{\partial T_j}{\partial z} &= \frac{T_j(j) - T_j(j-1)}{\Delta z}
\end{align*} \]