458.308 Process Control & Design

Lecture 2: Dynamic Modeling
- Theoretical (or Fundamental) Models

$$\dot{x} = f(x, u, p)$$

$$y = g(x, u, p)$$

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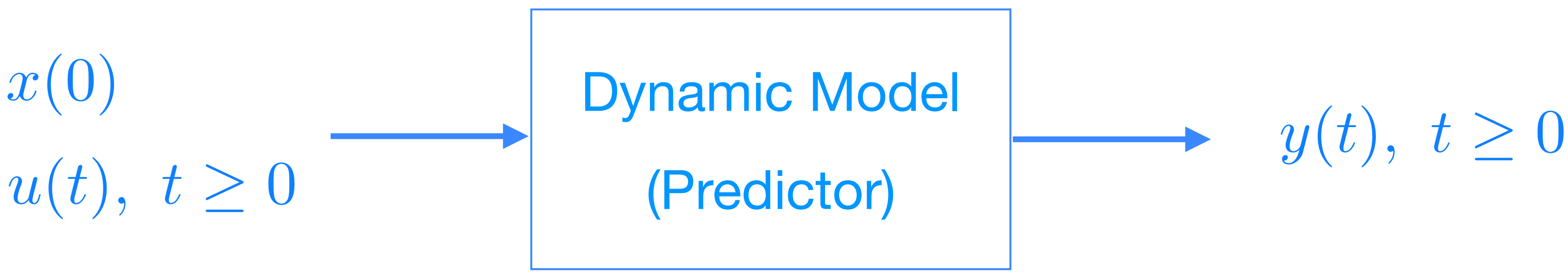
Objectives

- Write balance equations using instantaneous methods
- Incorporate appropriate constitutive relationships into the equations
- Determine the state, input, and output variables and the parameters
- Degrees of freedom analysis

Dynamic Modeling

Express the process's ______________

- Non steady-state initial condition, parameter changes, disturbances, etc.
- Often in the form of mathematical equation (time differential equation)



Why Dynamic Modeling?

Process dynamics must be understood well (often at a quantitative level) in order to design and operate the process effectively (e.g., design an effective control system)

Usage:

- Design (esp. batch processes, cyclic continuous processes that are inherently dynamic)
- Operability assessment (stability of intended operating condition, sensitivity to disturbances)
- Operator training
- Process optimization
- Design of startup / shutdown / transition procedure
- Design of control system

Modeling Approaches

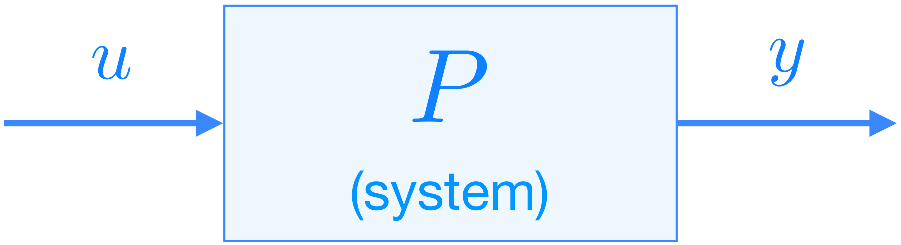
Fundamental Modeling

- Theoretical/Mechanistic modeling
- Physico-chemical understanding + Conservation principle
- Difficult to develop: need detailed process knowledge
- Usually complex: a large set of ODEs or PDEs
- Fundamentally correct - can be used for exploratory purposes
- Used for simulation (operator training), optimization, and transition control

Empirical Modeling

- Explain the observed response, cause-effect, pattern, etc.
- Easier to develop: need experimental data
- Usually kept simple: a small set of linear ODEs
- Lacks fundamental correctness: may not be useful in applications that require extrapolation beyond the conditions under which data were collected
- Used for controller design

Linear System



System can be seen as a mapping between input u and output y

Linear system should satisfy principle of superposition

This also implies ________

Principle of superposition

$$y = P(u), \; u \in \mathcal{D}, \; y \in \mathcal{R}$$

Consider $u_1, \; u_2 \in \mathcal{D} \longrightarrow y_1 = P(u_1), \; y_2 = P(u_2)$

For any scalar values of *a* and *b*:

$$P(au_1 + bu_2) = aP(u_1) + bP(u_2) = ay_1 + by_2$$

Determine if the systems given below are linear or not

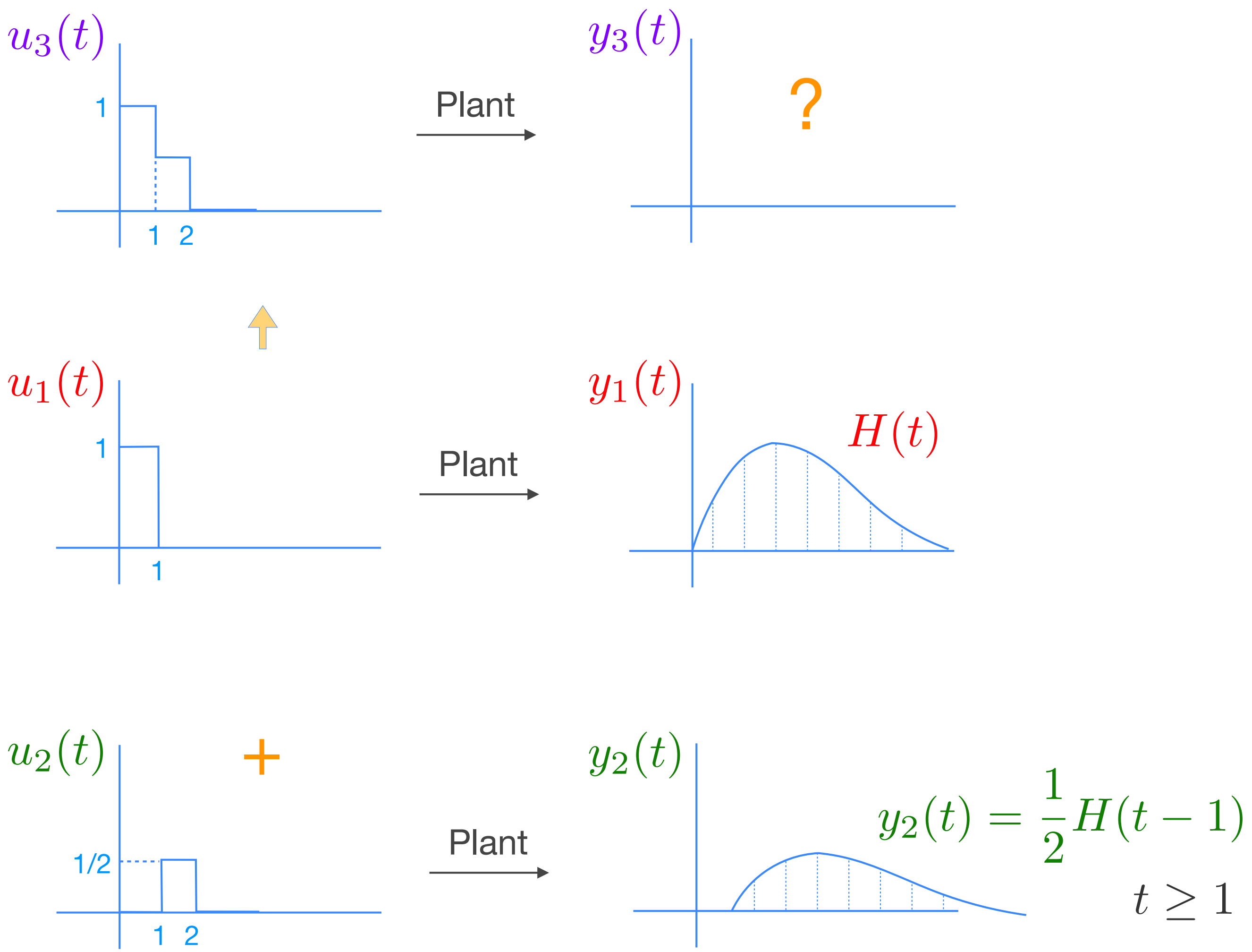
1. $y = 3u$

2. $y = 3u + 2$

3. Can you make (System 2) a linear system by defining a deviation variable?

Note: People often call affine system linear system

Advantage of Superposition Principle



Linear vs. Nonlinear Dynamics

- Linear model represents significant simplification
  - Knowledge of the output response to one particular input change can be extrapolated to predict the output responses to many different (sometimes any) input changes.
  - Gives approximate behavior (locally valid around some particular operating point) for most nonlinear processes. In this case, variables must be expressed in terms of **deviations from the steady-state values at the chosen operating point**
- Nonlinear Dynamic System: Any system that is NOT linear

How can you tell if a differential equation is linear or not?

If all the terms appear in the equation are linear functions of variables, it is linear. Otherwise it is not.

Linear

$$\frac{dy}{dt} + 3y = 2u(t)$$

$$a_n \frac{d^n y}{dt^n} + a_{n-1}\frac{d^{n-1}y}{dt^{n-1}} + \cdots a_1 \frac{dy}{dt} = bu(t)$$

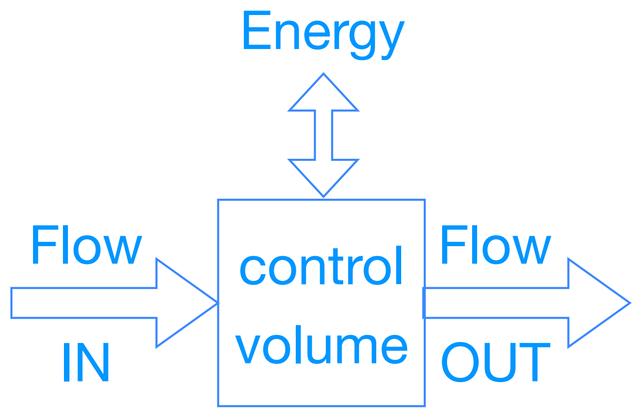
Nonlinear

$$\frac{dy}{dt} + y \sin y = 2u(t)$$

$$\frac{d^2y}{dt^2} + 3\frac{dy}{dt} + 2e^{-y} = u(t)$$

$$\frac{dy}{dt}y + \frac{d^2y}{dt^2} + y^3 = 3u(t)$$

Modeling Principle



1. Total mass balance

$$\begin{bmatrix} \text{Rate of} \\ \text{mass accumulation} \\ \text{within CV} \end{bmatrix} = \begin{bmatrix} \text{Rate of} \\ \text{mass in} \\ \text{from surroundings} \end{bmatrix} - \begin{bmatrix} \text{Rate of} \\ \text{mass out} \\ \text{to surroundings} \end{bmatrix}$$

2. Component mass (molar) balance

$$\begin{bmatrix} \text{Rate of component} \\ \text{mass accumulation} \\ \text{within CV} \end{bmatrix} = \begin{bmatrix} \text{Rate of component} \\ \text{mass in} \\ \text{from surroundings} \end{bmatrix} - \begin{bmatrix} \text{Rate of component} \\ \text{mass out} \\ \text{to surroundings} \end{bmatrix} + \begin{bmatrix} \text{Rate of component} \\ \text{mass creation} \\ \text{within CV} \end{bmatrix}$$

Modeling Principle

3. Total energy balance

$$\begin{bmatrix} \text{Rate of} \\ \text{energy accumulation} \\ \text{within CV} \end{bmatrix} = \begin{bmatrix} \text{Rate of} \\ \text{energy in} \\ \text{from surroundings} \end{bmatrix} - \begin{bmatrix} \text{Rate of} \\ \text{energy out} \\ \text{to surroundings} \end{bmatrix}$$

For flow systems,

$$\begin{bmatrix} \text{Rate of} \\ \text{enthalpy accumulation} \\ \text{within CV} \end{bmatrix} = \begin{bmatrix} \text{Rate of} \\ \text{enthalpy in} \\ \text{by material flow} \end{bmatrix} - \begin{bmatrix} \text{Rate of} \\ \text{enthalpy out} \\ \text{by material flow} \end{bmatrix} + \begin{bmatrix} \text{Rate of total} \\ \text{heat addition} \\ \text{from surroundings} \end{bmatrix}$$

4. Total momentum balance

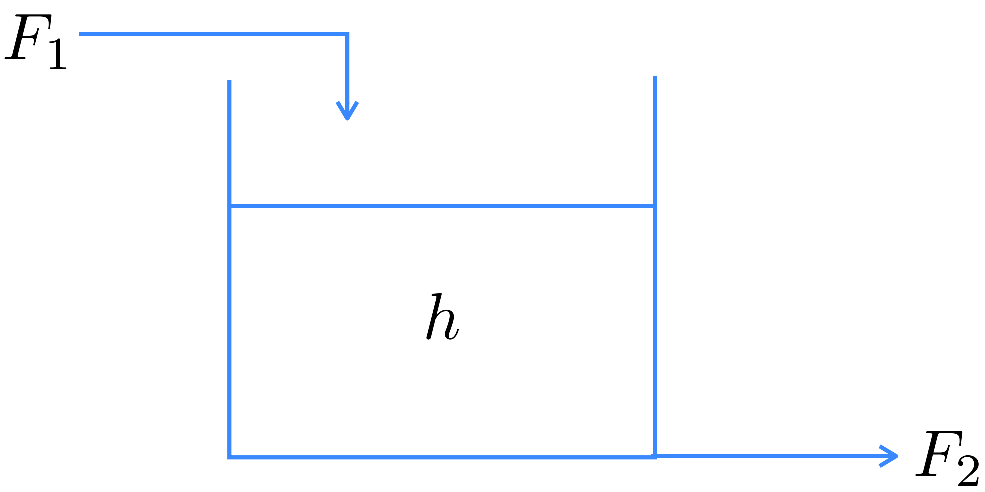
$$\begin{bmatrix} \text{Rate of} \\ \text{momentum (mv) accumulation} \\ \text{within CV} \end{bmatrix} = \begin{bmatrix} \text{Net force} \\ \text{working} \\ \text{on CV} \end{bmatrix}$$

Modeling Procedure

1. Draw the control volume (Inside C.V., all intrinsic properties should be assumed same)
2. Identify which balances are necessary
    - Changing volume, height: Total Mass Balance
    - Changing concentration: Component mass or molar balance
    - Changing temperature: Energy balance
3. Write down mathematical expression for each term
4. Put them together into equation
5. Incorporate constitutive equations if needed
6. Use the chain rule, etc. to simplify

Examples of Mass Balance

1. Surge Tank



Given

ρ : liquid density

A : cross-sectional area of vessel

$F_1, \; F_2$: volumetric flow rate (vol./time)

Total M.B.

Total mass inside CV: $m = \rho V$

Rate of mass accumulation inside CV: $\dfrac{d(\rho V)}{dt}$

Rate of mass into CV by flow: ρF_1

Rate of mass out of CV by flow: ρF_2

$$\frac{d(\rho V)}{dt} = \rho F_1 - \rho F_2 \quad \text{---} \; (1)$$

Constitutive Equation?

$$V = Ah \quad \text{-------------} \quad (2)$$

(2) → (1)

$$\frac{d(\rho A h)}{dt} = \rho F_1 - \rho F_2$$

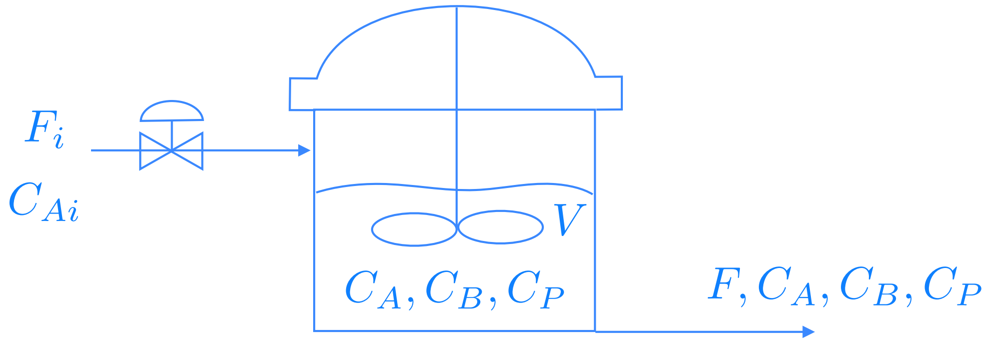
If ρ and A are constants,

$$\rho A \frac{dh}{dt} = \rho F_1 - \rho F_2$$

state variable: h
input variables: $F_1, \; F_2$
output variable: h
parameter: A

Ethylene oxide (A) is reacted with water (B) in a CSTR to form ethylene glycol (P): A + B → P. Assume the temperature is maintained at a constant value and that the water is in large excess. Also assume that $\rho_i = \rho$

Develop a model to find the concentration for each species as a function of time.



Total Mass Balance

$$\frac{d(\rho V)}{dt} = \rho_i F_i - \rho F \longrightarrow \boxed{\frac{dV}{dt} = F_i - F} \quad (1)$$

note: $\frac{dV}{dt} \neq 0$

Component Mass Balances $C_A,\ C_B,\ C_P \ \left[\frac{\text{moles}}{\text{vol}}\right]$

$$A: \frac{d(VC_AM_A)}{dt} = F_iC_{Ai}M_A - FC_AM_A + r_A \cdot V \cdot M_A \qquad (2)$$

M_A : molecular weight [mass/mol]

Similarly,

$$P: \frac{d(VC_p)}{dt} = 0 - FC_P + r_pV \qquad (3)$$

Constitutive equations:

$$r_A = -kC_A,\ r_p = kC_A \qquad (4)$$

(4) → (2) (3)

$$\frac{d(VC_A)}{dt} = F_i C_{Ai} - FC_A - VkC_A \quad \text{(2')}$$

$$\frac{d(VC_P)}{dt} = -FC_P + VkC_A \quad \text{(3')}$$

(2')

$$\frac{d(VC_A)}{dt} = V\frac{dC_A}{dt} + C_A\frac{dV}{dt}$$

$$= V\frac{dC_A}{dt} + C_A(F_i - F)$$ LHS

$$= F_i C_{Ai} - FC_A - VkC_A$$ RHS

⇨

⇨ (2'')

Similarly, (3') becomes

$$\frac{dC_P}{dt} = -\frac{F_i}{V} C_P + kC_A \qquad (3'')$$

State Variables

$$x = \begin{bmatrix} V \\ C_A \\ C_P \end{bmatrix}$$

Input Variables

$$u = \begin{bmatrix} F_i \\ F \\ C_{Ai} \end{bmatrix}$$

Parameters

$$p = [k]$$

Energy Balance

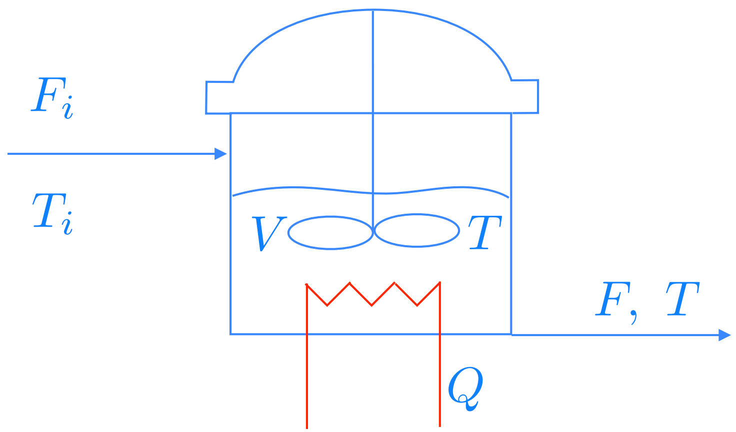
Preliminary

TE (total energy) = U (internal) + KE (kinetic) + PE (potential)

negligible compared to thermal energy

For flow systems: H = U + pV

Stirred Tank Heater



Assume

F_i, T_i can vary

Tank is insulated

Q (rate of heat added per time) can vary

Develop a model to find the tank liquid temperature as a function of time

Material Balance

$$\frac{d(V\rho)}{dt} = F_i\rho_i - F\rho$$

Energy Balance

$$\frac{dTE}{dt} = F_i\rho_i T\hat{E}_i - F\rho T\hat{E} + Q + W_T$$

work done on the system

We neglect the kinetic and potential energy:

$$\frac{dU}{dt} = F_i\rho_i\hat{U}_i - F\rho\hat{U} + Q + W_T$$

$$W_T = W_s + F_i p_i - Fp$$

$$\frac{dU}{dt} = F_i\rho_i\left(\hat{U}_i + \frac{p_i}{\rho_i}\right) - F\rho\left(\hat{U}_i + \frac{p}{\rho}\right) + Q + W_s$$

neglect the mean pressure change (liquid)

$$\frac{dH}{dt} - \frac{dpV}{dt} = F_i\rho_i\hat{H}_i - F\rho\hat{H} + Q + W_s$$

$$\frac{dpV}{dt} = V\frac{dp}{dt} + p\frac{dV}{dt}$$

constant volume

Assume that the heat capacity is constant (hence, no phase change)

$$\frac{d[V\rho c_p(T - T_{ref})]}{dt} = F_i \rho_i c_p (T_i - T_{ref}) + Q - F\rho c_p (T - T_{ref}) + W_s$$

Assume constant density and volume (hence, $F_i = F$)

$$\frac{d[V\rho c_p(T - T_{ref})]}{dt} = F\rho c_p \left[(T_i - T_{ref}) - (T - T_{ref})\right] + Q + W_s$$

Note

state: T

inputs: F, T_i, Q

parameters: V, ρ, c_p

Linear? Nonlinear? Examples We Worked on

Surge Tank

$$\frac{dh}{dt} = \frac{F_1 - F_2}{A} \quad \Longleftrightarrow \quad \frac{dy}{dt} = \frac{u_1 - u_2}{A}$$

CSTR (constant hold-up)

$$\frac{dC_A}{dt} = \frac{F_i}{V}(C_{Ai} - C_A) - kC_A$$

$$\Longleftrightarrow \quad \frac{dy}{dt} = \frac{u_1}{V}(u_2 - y) - ky$$

Degrees of Freedom Analysis

DoF: Number of variables that can be specified independently

$$\mathbf{N}_F = \mathbf{N}_V - \mathbf{N}_E$$

$\mathbf{N}_F$: Degree of freedom (# of independent variables)

$\mathbf{N}_V$: Total number of variables

$\mathbf{N}_E$: Number of equations (# of dependent variables)

Another perspective: # of equations needed?

$$\mathbf{N}_E = \mathbf{N}_V - \mathbf{N}_F$$

DoF: Heated Tank Example

$$\frac{dT}{dt} = \frac{F}{V}(T_i - T) + \frac{Q}{V\rho c_p}$$

state: T

inputs: F, T_i, Q

parameters: V, ρ, c_p

Lumped Parameter System

- Spatial dependence of variables is ignored
  - Well-mixed system
  - Systems with insignificant temperature or concentration gradient
  - Variables are functions of time only, not spatial position
  - Ordinary differential equation model
- Examples
  - Mixer, CSTR
  - Tray of distillation column
  - Steel ball for which heat conduction within much faster than heat transfer to the surrounding

Distributed Parameter System

- Variables have spatial dependence
  - Instead of $y(t)$, you have $y(t, z)$, $y(t, r, z)$, etc.
- Type of equation
  - PDEs
- Examples
  - Counter-current heat exchanger
  - Plug-flow reactor or packed-tube reactor
  - Heat conduction through a plate
  - Almost all systems show some spatial variations (e.g., due to imperfect mixing) but many systems can be treated as lumped parameter system