458.308 Process Control & Design

Lecture 2: Dynamic Modeling

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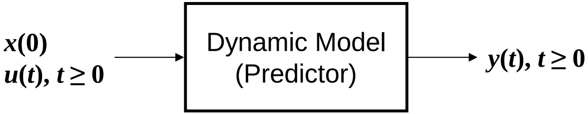
Dynamic Modeling

Express the process's time behaviour

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



$x(0)$: initial "state"
$u(t)$: time behaviour of some parameter (independent variable)

$y(t)$: time behaviour of (dependent) variables of interest

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

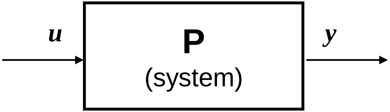
Fundamental Modeling

- 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...

- $P(0) = 0$

Principle of superposition

$y = P(u)$, $u \in \mathcal{D}$, $y \in \mathcal{R}$
Consider $u_1,\ u_2\ \in \mathcal{D}$
$y_1 = P(u_1),\ y_2 = P(u_2)$
for any scalar values of $a,\ b$

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

Affine System

- Q. $y = 3u$?
- A.
- Q. $y = 3u + 2$?
- A.
- Q. Deviation variable?
- A.

Note: People often call affine system linear system.

Linear? Nonlinear?: Examples We Worked on

- Surge Tank

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

- CSTR (constant hold-up)

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

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

Degree 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 independent variables)

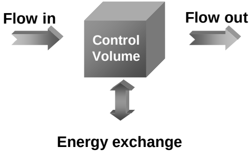
- Another perspective: # of equations needed?

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

Stirred-Tank Heating Process

- $\mathbf{N}_V = 6$: $T_i,\ w_i,\ T,\ w,\ V,\ Q$
- $\mathbf{N}_E = 2$: mass and energy balances
- $\mathbf{N}_F = N_V - N_E = 4$
- If we have constant holdup and $w = w_i$
  - $\mathbf{N}_V = 4$
  - $\mathbf{N}_E = 1$: Only energy balance
  - $\mathbf{N}_F = 3$: Three independent variables would be $T_i,\ w,\ Q$

General Modeling Principle



- Total mass balance
  - Rate of mass accumulation within CV = Rate of mass in from surroundings - Rate of mass out to surroundings
- Component mass (molar) balance
  - Rate of mass accumulation within CV = Rate of mass in from surroundings - Rate of mass out to surroundings + Rate of mass creation within CV
- Total energy (enthalpy) balance
  - Rate of energy accumulation within CV = Rate of energy in from surroundings - Rate of energy out to surroundings
  - For flow systems,

    Rate of enthalpy accumulation within CV = Rate of enthalpy in by material flow - Rate of enthalpy out by material flow + Rate of total heat addition from surroundings

Illustrative Example: Stirred-Tank Heating Process

Total mass inside CV = $V\rho$
Rate of mass accumulation inside CV = $\frac{d(V\rho)}{dt}$
Rate of mass into CV by flow = w_i
Rate of mass out of CV by flow = w
Total energy inside CV = $H = \rho V\hat{H}$
Rate of energy into CV by flow = $w_i\hat{H}_i = w_i C(T_i - T_{ref})$
Rate of energy out of CV by flow = $w\hat{H} = w_i C(T - T_{ref})$

Rate of energy addition = Q

$$
\begin{aligned}
\frac{dV}{dt} &= \frac{1}{\rho}(w_i - w) \\
\frac{dT}{dt} &= \frac{w_i}{V\rho}(T_i - T) + \frac{Q}{\rho VC}
\end{aligned}
$$

Note: Several additional examples are available in the textbook. To become good at modeling, you must try many different problems on your own.

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 is much faster than heat transfer to the surrounding

Distributed Parameter System

- Variables have spatial dependence
  - Instead of $y(t)$, you have $y(t,\ z)$, $y(t,\ r,\ z)$, or $y(t,\ r,\ z,\ \theta)$.
- Type of equation
  - Lumped parameter system $\Rightarrow$ ODEs
  - Distributed parameter system $\Rightarrow$ PDEs
- Example
  - 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 impperfect mixing) but many systems can be treated as lumped parameter system.