

458.308 Process Control & Design

Lecture 3: Dynamic Simulation and Analysis

Jong Min Lee

Chemical & Biomolecular Engineering
Seoul National University

Standard Form of the Model

2 dependent variables and 2 independent variables

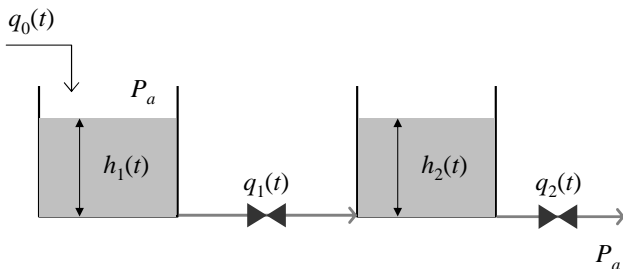
$$\dot{x}_1 = f_1(x_1, x_2, u_1, u_2)$$

$$\dot{x}_2 = f_2(x_1, x_2, u_1, u_2)$$

f_1, f_2 : some (nonlinear) functions of x_1, x_2, u_1, u_2

- There can be many more dependent variables and many more independent variables. What would be the form with n dependent variables and m independent variables?

Example: Interacting Tanks



$$q_1 = C'_{v1} \sqrt{(P_a + \rho g h_1) - (P_a + \rho g h_2)} = C'_{v1} \sqrt{\rho g (h_1 - h_2)} = C_{v1} \sqrt{h_1 - h_2}$$

$$q_2 = C'_{v2} \sqrt{(P_a + \rho g h_2) - P_a} = C'_{v2} \sqrt{\rho g h_2} = C_{v2} \sqrt{h_2}$$

Standard Form

$$\frac{d(A_1 h_1 \rho)}{dt} = \rho q_0 - \underbrace{\rho C_{v1} \sqrt{h_1 - h_2}}_{q_1}$$

$$\frac{d(A_2 h_2 \rho)}{dt} = \underbrace{\rho C_{v1} \sqrt{h_1 - h_2}}_{q_1} - \underbrace{\rho C_{v2} \sqrt{h_2}}_{q_2}$$

$$x_1 \triangleq h_1, \quad x_2 \triangleq h_2, \quad u_1 \triangleq q_0$$

$$\underbrace{\frac{dh_1}{dt}}_{\dot{x}_1} = \underbrace{\frac{q_0 - C_{v1} \sqrt{h_1 - h_2}}{A_1}}_{f_1(x_1, x_2, u_1)}$$

$$\underbrace{\frac{dh_2}{dt}}_{\dot{x}_2} = \underbrace{\frac{C_{v1} \sqrt{h_1 - h_2} - C_{v2} \sqrt{h_2}}{A_2}}_{f_2(x_1, x_2, u_1)}$$

What can you do with the model?

- **Numerical integration** ("simulation") to investigate the time behaviour of the dependent variables to a particular $x(0)$ (initial condition) and $u(t)$, $t \geq 0$ (independent variable).
 - What does "numerical solving" the ODEs mean?
 - Given: $x(0)$ and $u(t)$, $t \geq 0$
 - Obtain: $x(t)$, $t \geq 0$
- **Analysis**
 - Linearization
 - Analytical solution via Laplace Transform

Numerical Integration

- 1 Start with $x_1(0)$ and $x_2(0)$. Set $t = 0$.
- 2 Take an incremental step (of size Δt , which cannot be large, why?) forward in time by solving

- Forward Euler: Explicit integration

$$x_1(t + \Delta t) = x_1(t) + \Delta t \cdot f_1(x_1(t), \dots)$$

$$x_2(t + \Delta t) = x_2(t) + \Delta t \cdot f_2(x_1(t), \dots)$$

- Backward Euler: Implicit Integration

$$x_1(t + \Delta t) = x_1(t) + \Delta t \cdot f_1(x_1(t + \Delta t), \dots)$$

$$x_2(t + \Delta t) = x_2(t) + \Delta t \cdot f_2(x_1(t + \Delta t), \dots)$$

- Trapezoidal (2nd order R-K): Implicit Integration

$$x_1(t + \Delta t) = x_1(t) + \Delta t \cdot \frac{f_1(x_1(t), \dots) + f_1(x_1(t + \Delta t), \dots)}{2}$$

$$x_2(t + \Delta t) = x_2(t) + \Delta t \cdot \frac{f_2(x_1(t), \dots) + f_2(x_1(t + \Delta t), \dots)}{2}$$

- 3 Repeat this until you reach the desired end time.

Equilibrium Calculation

- At steady state, $d/dt = 0$

$$0 = f_1(\bar{x}_1, \bar{x}_2, \bar{u}_1, \bar{u}_2)$$

$$0 = f_2(\bar{x}_1, \bar{x}_2, \bar{u}_1, \bar{u}_2)$$

- Given the steady state values of **the independent variables**, one can calculate the corresponding steady-state values of the dependent values by solving the above equation.

Solving Algebraic Equations Numerically

Newton Iteration

$$\begin{aligned} \begin{bmatrix} 0 \\ 0 \end{bmatrix} &= \begin{bmatrix} f_1(\bar{x}_1, \bar{x}_2) \\ f_2(\bar{x}_1, \bar{x}_2) \end{bmatrix} \\ &\approx \begin{bmatrix} f_1(\bar{x}_1^i, \bar{x}_2^i) \\ f_2(\bar{x}_1^i, \bar{x}_2^i) \end{bmatrix} + \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{bmatrix}_{(\bar{x}_1^i, \bar{x}_2^i)} \begin{bmatrix} \bar{x}_1 - \bar{x}_1^i \\ \bar{x}_2 - \bar{x}_2^i \end{bmatrix} \end{aligned}$$

\bar{x}^i : current guess of the solutions

By solving the above approximate equation, one gets iterative formula:

$$\begin{bmatrix} \bar{x}_1^{i+1} \\ \bar{x}_2^{i+1} \end{bmatrix} = \begin{bmatrix} \bar{x}_1^i \\ \bar{x}_2^i \end{bmatrix} - \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{bmatrix}_{(\bar{x}_1^i, \bar{x}_2^i)}^{-1} \begin{bmatrix} f_1(\bar{x}_1^i, \bar{x}_2^i) \\ f_2(\bar{x}_1^i, \bar{x}_2^i) \end{bmatrix}$$

Example

$$0 = \bar{q}_0 - C_{v1} \sqrt{\rho g (\bar{h}_1 - \bar{h}_2)}$$

$$0 = C_{v1} \sqrt{\rho g (\bar{h}_1 - \bar{h}_2)} - C_{v2} \sqrt{\rho g \bar{h}_2}$$

$$\begin{bmatrix} \bar{h}_1^{i+1} \\ \bar{h}_2^{i+1} \end{bmatrix} = \begin{bmatrix} \bar{h}_1^i \\ \bar{h}_2^i \end{bmatrix} - M_i^{-1} \begin{bmatrix} \bar{q}_0 - C_{v1} \sqrt{\rho g (\bar{h}_1^i - \bar{h}_2^i)} \\ C_{v1} (\bar{h}_1^i - \bar{h}_2^i) - C_{v2} \sqrt{\rho g \bar{h}_2^i} \end{bmatrix}$$

$$M_i = \begin{bmatrix} -\frac{C_{v1} \sqrt{\rho g}}{2\sqrt{(\bar{h}_1^i - \bar{h}_2^i)}} & \frac{C_{v1} \sqrt{\rho g}}{2\sqrt{(\bar{h}_1^i - \bar{h}_2^i)}} \\ \frac{C_{v1} \sqrt{\rho g}}{2\sqrt{(\bar{h}_1^i - \bar{h}_2^i)}} & -\frac{C_{v1} \sqrt{\rho g}}{2\sqrt{(\bar{h}_1^i - \bar{h}_2^i)}} - \frac{C_{v2} \sqrt{\rho g}}{2\sqrt{\bar{h}_2^i}} \end{bmatrix}$$

Linearization: 1st Order Approximation of ODEs Around an Equilibrium

$$\dot{x}_1 = f_1(x_1, x_2, u_1, u_2)$$

$$\dot{x}_2 = f_2(x_1, x_2, u_1, u_2)$$

1st-order Taylor series expansion at the equilibrium

$(\bar{x}_1, \bar{x}_2, \bar{u}_1, \bar{u}_2)$

$$\begin{aligned} \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} &\approx \begin{bmatrix} f_1(\bar{x}_1, \bar{x}_2, \bar{u}_1, \bar{u}_2) \\ f_2(\bar{x}_1, \bar{x}_2, \bar{u}_1, \bar{u}_2) \end{bmatrix} + \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{bmatrix}_{(\bar{x}_1, \bar{x}_2, \bar{u}_1, \bar{u}_2)} \begin{bmatrix} x_1 - \bar{x}_1 \\ x_2 - \bar{x}_2 \end{bmatrix} \\ &+ \begin{bmatrix} \frac{\partial f_1}{\partial u_1} & \frac{\partial f_1}{\partial u_2} \\ \frac{\partial f_2}{\partial u_1} & \frac{\partial f_2}{\partial u_2} \end{bmatrix}_{(\bar{x}_1, \bar{x}_2, \bar{u}_1, \bar{u}_2)} \begin{bmatrix} u_1 - \bar{u}_1 \\ u_2 - \bar{u}_2 \end{bmatrix} \end{aligned}$$

Linearized Model

Standard Form: 2×2 System

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} \approx \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{bmatrix}_{(\bar{x}_1, \bar{x}_2, \bar{u}_1, \bar{u}_2)} \begin{bmatrix} x_1 - \bar{x}_1 \\ x_2 - \bar{x}_2 \end{bmatrix} + \begin{bmatrix} \frac{\partial f_1}{\partial u_1} & \frac{\partial f_1}{\partial u_2} \\ \frac{\partial f_2}{\partial u_1} & \frac{\partial f_2}{\partial u_2} \end{bmatrix}_{(\bar{x}_1, \bar{x}_2, \bar{u}_1, \bar{u}_2)} \begin{bmatrix} u_1 - \bar{u}_1 \\ u_2 - \bar{u}_2 \end{bmatrix}$$

Deviation variables: $x'_1 \equiv x_1 - \bar{x}_1$, etc.

$$\begin{bmatrix} \dot{x}'_1 \\ \dot{x}'_2 \end{bmatrix} = A \begin{bmatrix} x'_1 \\ x'_2 \end{bmatrix} + B \begin{bmatrix} u'_1 \\ u'_2 \end{bmatrix}$$

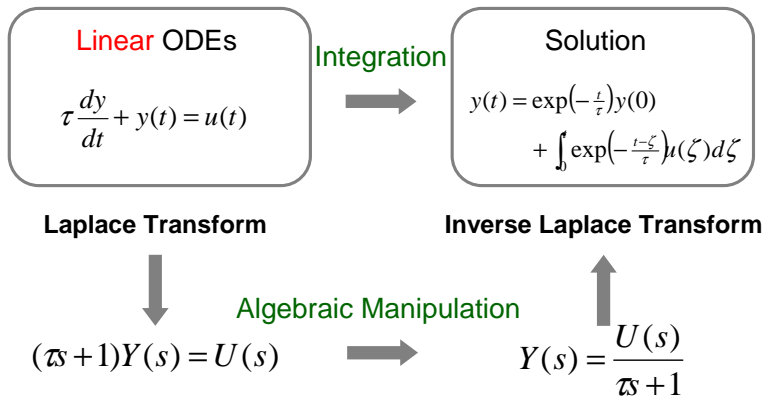
Example

$$\underbrace{\frac{dh_1}{dt}}_{\dot{x}_1} = \underbrace{\frac{q_0 - C_{v1}\sqrt{h_1 - h_2}}{A_1}}_{f_1(x_1, x_2, u_1)}$$
$$\underbrace{\frac{dh_2}{dt}}_{\dot{x}_2} = \underbrace{\frac{C_{v1}\sqrt{h_1 - h_2} - C_{v2}\sqrt{h_2}}{A_2}}_{f_2(x_1, x_2, u_1)}$$

Linearization at $\bar{h}_1, \bar{h}_2, \bar{q}_0$

$$\begin{bmatrix} \frac{dh'_1}{dt} \\ \frac{dh'_2}{dt} \end{bmatrix} = \begin{bmatrix} -\frac{C_{v1}}{2A_1\sqrt{\bar{h}_1 - \bar{h}_2}} & \frac{C_{v1}}{2A_1\sqrt{\bar{h}_1 - \bar{h}_2}} \\ \frac{C_{v1}}{2A_2\sqrt{\bar{h}_1 - \bar{h}_2}} & -\frac{C_{v1}}{2A_2\sqrt{\bar{h}_1 - \bar{h}_2}} - \frac{C_{v2}}{2A_2\sqrt{\bar{h}_2}} \end{bmatrix} \begin{bmatrix} h'_1 \\ h'_2 \end{bmatrix} + \begin{bmatrix} \frac{1}{A_1} \\ 0 \end{bmatrix} q'_0$$

Laplace Transform -- Main Idea



Laplace Transform -- Key Points

Definition

$$F(s) = \mathcal{L}[f(t)] = \int_0^{\infty} f(t) e^{-st} dt$$

- Laplace Transform for simple signals
 - Steps, ramps, exponential decay or rise, pulse, impulse, etc.
 - Can be found by evaluating the integral
 - See Table 3.1
 - Must memorize the simple ones

Important Properties

$$\mathcal{L}\left(\frac{df}{dt}\right) = sF(s) - f(0)$$

$$\mathcal{L}\left(\frac{d^2f}{dt^2}\right) = s^2F(s) - sf(0) - f'(0)$$

$$\mathcal{L}\left(\int_0^t f(\zeta) d\zeta\right) = \frac{1}{s}F(s)$$

$$\mathcal{L}(f(t - \delta)) = F(s)e^{-\delta s}$$

Key Points

Warning: LT is a linear operation!

$$\mathcal{L}(af_1(t) + bf_2(t)) = aF_1(s) + bF_2(s)$$

$$\mathcal{L}(y^2(t)) \neq Y^2(s)$$

$$\mathcal{L}(y(t)u(t)) \neq Y(s)U(s)$$

Final and Initial Value Theorem

$$\lim_{t \rightarrow \infty} f(t) = \lim_{s \rightarrow 0} sF(s)$$

$$f(0) = \lim_{s \rightarrow \infty} sF(s)$$

Inverse Laplace Transform

- Needed to take the solution obtained through Laplace transform back to the time domain.
- The formula involves complex contour integral.
- Use **partial fraction** expansion to break the solution down to small pieces and use the table (or your memory) to invert.
 - 1 Break down $X(s)$ into sum of fractions

$$X(s) = \frac{A_1}{s - p_1} + \frac{A_2}{s - p_2} + \cdots + \frac{A_m}{s - p_m}$$

- 2 Using linearity property, write

$$\begin{aligned}x(t) &= \mathcal{L}^{-1}\{X(s)\} = \mathcal{L}^{-1}\left\{\frac{A_1}{s - p_1}\right\} + \mathcal{L}^{-1}\left\{\frac{A_2}{s - p_2}\right\} + \cdots + \mathcal{L}^{-1}\left\{\frac{A_m}{s - p_m}\right\} \\ &= A_1 e^{p_1 t} + A_2 e^{p_2 t} + \cdots + A_m e^{p_m t}\end{aligned}$$

Transfer Function

- **Linear differential equation** with a general forcing function (input)

1st order $a \frac{dy}{dt} + y(t) = Ku(t)$

2nd order $b \frac{d^2y}{dt^2} + a \frac{dy}{dt} + y(t) = Ku(t)$

...

- We can solve the eqn. for a specific forcing function, but we can also leave it general and take Laplace transform (with the initial condition zero!) to arrive at a **general relationship between output and input**.

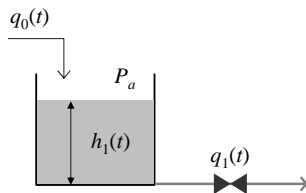
$$Y(s) = \frac{K}{as + 1} U(s); \quad Y(s) = \frac{K}{bs^2 + as + 1} U(s)$$

- With the transfer function, one can conveniently calculate the response of the output to any input by **multiplication**.

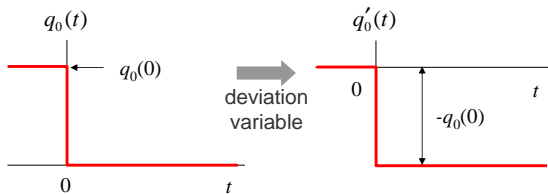
$$Y(s) = G(s) U(s)$$

Single-Tank Draining

Assume that you start at the steady state: $q_0(0) = \bar{q}_0$, $h_1(0) = \bar{h}_1$



$$q_1 = C_{v1} \sqrt{P_a + \rho g h_1 - P_a} = C_{v1} \sqrt{\rho g h_1} = C_{v1} \sqrt{h_1}$$



Mass Balances

$$\frac{d(A_1 h_1 \rho)}{dt} = \rho q_0 - \underbrace{\rho C_{v1} \sqrt{h_1}}_{q_1}$$

Q. Do you think you can solve the above using L.T.?

A. No.

Linearize!

$$A_1 \frac{dh'_1}{dt} = q'_0 - \underbrace{\left(\frac{C_{v1}}{2\sqrt{h_1}} \right)}_{1/R_1} h'_1$$

Note: The above can be solved (using L.T.) but will the linear model be valid throughout the entire draining experiment?

Solution Based on the **Linearized** Model

$$A_1 \frac{dh'_1}{dt} = q'_0 - \frac{1}{R_1} h'_1 \text{ with } h'_1(0) = 0, q'_0(s) = -\frac{\bar{q}_0}{s}$$

$$\Downarrow \mathcal{L}$$

$$\left(A_1 s + \frac{1}{R_1} \right) H_1(s) = -\frac{\bar{q}_0}{s}, H_1(s) = \frac{-\bar{q}_0 R_1}{s} + \frac{\bar{q}_0 R_1}{s + \frac{1}{A_1 R_1}}$$

$$\Downarrow \mathcal{L}^{-\infty}$$

$$h'_1(t) = -\bar{q}_0 R_1 \left(1 - \exp\left(-\frac{t}{A_1 R_1}\right) \right)$$

†Note: We can see that $h_1(t)$ is an exponentially decaying function of t .

Real Solution

Integrate the differential equation from time 0 to t to obtain

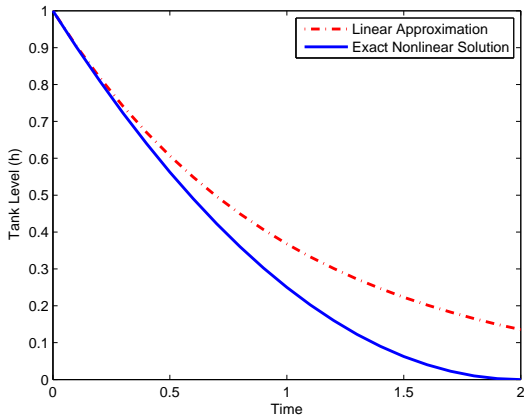
$$A_1 \frac{dh_1'}{dt} = -C_{v1} \sqrt{h_1}, \quad h(0) = \bar{h}$$
$$\frac{1}{\sqrt{h_1}} \frac{dh_1}{dt} = -\frac{C_{v1}}{A_1}$$

↓

$$2 \left(\sqrt{h_1(t)} - \sqrt{\bar{h}_1} \right) = \frac{-C_{v1}}{A_1} (t - 0)$$
$$h_1(t) = \left(\frac{-C_{v1}}{2A_1} t + \sqrt{\bar{h}_1} \right)^2$$

†Note: We can see that $h_1(t)$ is a quadratic function of t .

Comparison



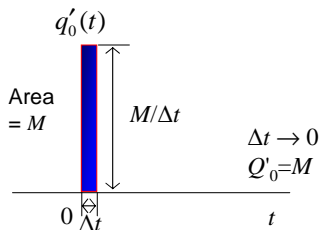
Interacting Tanks -- Revisited

$$\begin{bmatrix} \frac{dh'_1}{dt} \\ \frac{dh'_2}{dt} \end{bmatrix} = \begin{bmatrix} -\frac{1}{A_1 R_1} & \frac{1}{A_1 R_1} \\ \frac{1}{A_2 R_1} & -\frac{1}{A_2} \left(\frac{1}{R_1} + \frac{1}{R_2} \right) \end{bmatrix} \begin{bmatrix} h'_1 \\ h'_2 \end{bmatrix} + \begin{bmatrix} \frac{1}{A_1} \\ 0 \end{bmatrix} q'_0$$

$\Downarrow \quad \mathcal{L}$

$$\begin{bmatrix} H'_1(s) \\ H'_2(s) \end{bmatrix} = \begin{bmatrix} \frac{\left(s + \frac{1}{A_2} \left(\frac{1}{R_1} + \frac{1}{R_2} \right) \right) \frac{1}{A_1}}{\left(s + \frac{1}{A_2} \left(\frac{1}{R_1} + \frac{1}{R_2} \right) \right) \left(s + \frac{1}{A_1 R_1} \right) - \frac{1}{A_1 A_2 R_1^2}} Q'_0(s) \\ \frac{\frac{1}{A_1 A_2 R_1}}{\left(s + \frac{1}{A_2} \left(\frac{1}{R_1} + \frac{1}{R_2} \right) \right) \left(s + \frac{1}{A_1 R_1} \right) - \frac{1}{A_1 A_2 R_1^2}} Q'_0(s) \end{bmatrix}$$

Impulse Response



$$\begin{bmatrix} H'_1(s) \\ H'_2(s) \end{bmatrix} = \begin{bmatrix} G_1(s) \cdot M \\ G_2(s) \cdot M \end{bmatrix} \quad \text{Inverse L.T.} \Rightarrow \begin{bmatrix} h'_1(t) \\ h'_2(t) \end{bmatrix}$$

Properties of Transfer Functions

- Steady-state gain: $G(0)$ -- Output change under a **unit step change** in input as $t \rightarrow \infty$
- The order of the denominator polynomial = the order of the equivalent differential equation
- Physical realizability: $n \geq m$

$$G(s) = \frac{Y(s)}{U(s)} = \frac{b_m s^m + b_{m-1} s^{m-1} + \dots + b_0}{a_n s^n + a_{n-1} s^{n-1} + \dots + a_0}$$

- **Additive** and **multiplicative** property