Lecture 3
Dynamic Modeling
Part III: Simulation and Analysis

CHE4400
Professor Jay H. Lee
Georgia Inst. Technology

Standard Form of the Model

- 2 dependent variables and two independent variables:

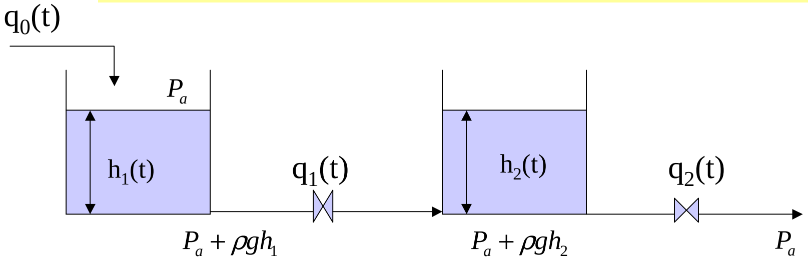
$$\begin{aligned}\dot{x}_1 &= f_1(x_1, x_2, u_1, u_2)\\ \dot{x}_2 &= f_2(x_1, x_2, u_1, u_2)\end{aligned}$$

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

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



$$q_2 = C_{v2}\sqrt{P_a+\rho g h_2 - P_a} = C_{v2}\sqrt{\rho g h_2}$$

Standard Form

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

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

⬇ where $x_1 \equiv h_1,\ x_2 \equiv h_2, u_1 \equiv q_0$

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

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

What can you do with the model?

- **Numerical integration** ("simulation") to investigate the time behavior of the dependent variables to a particular x(0) (initial condition) and u(t), t≥0 (independent variable).

  What does "numerically solving" the ODEs mean?
  - Given: x(0) and (u(t), t≥0)
  - Obtain (x(t), t>0)
- **Analysis:**
  - Linearization
  - Analytical solution via Laplace Transform

Numerical Integration

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

Forward Euler: ***Explicit*** *Integration*

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

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

Backward Euler: ***Implicit*** *Integration*

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

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

Trapezoidal (2^{nd} order R-K): ***Implicit*** *Integration*

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

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

- Repeat this until you reach the desired end time

Equilibrium Calculation

- At steady state, d/dt=0

$$
\begin{aligned}
0 &= f_1(\bar{x}_1, \bar{x}_2, \bar{u}_1, \bar{u}_2) \\
0 &= f_2(\bar{x}_1, \bar{x}_2, \bar{u}_1, \bar{u}_2)
\end{aligned}
$$

- 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

current guess of the solutions

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

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

$$0 = \bar{q}_0 - C_{v1}\sqrt{\rho g(\bar{h}_1 - \bar{h}_2)}$$
$$0 = C_{v1}\sqrt{\rho g(\bar{h}_1 - \bar{h}_2)} - C_{v2}\sqrt{\rho g\bar{h}_2}$$

$\bar{h}_1^0, \bar{h}_2^0$ ← Initial guess, i=0

Newton iteration (repeat until convergence!)

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

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

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

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

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} \approx \cancelto{0}{\begin{bmatrix} f_1(\bar{x}_1, \bar{x}_2, \bar{u}_1, \bar{u}_2) \\ f_2(\bar{x}_1, \bar{x}_2, \bar{u}_1, \bar{u}_2) \end{bmatrix}} + \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{bmatrix}_{(\bar{x}_1, \bar{x}_2, \bar{u}_1, \bar{u}_2)} \begin{bmatrix} x_1 - \bar{x}_1 \\ x_2 - \bar{x}_2 \end{bmatrix}$$
$$+ \begin{bmatrix} \frac{\partial f_1}{\partial u_1} & \frac{\partial f_1}{\partial u_2} \\ \frac{\partial f_2}{\partial u_1} & \frac{\partial f_2}{\partial u_2} \end{bmatrix}_{(\bar{x}_1, \bar{x}_2, \bar{u}_1, \bar{u}_2)} \begin{bmatrix} u_1 - \bar{u}_1 \\ u_2 - \bar{u}_2 \end{bmatrix}$$

Standard Form of Linearized Model

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

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

$\Downarrow$ $x_1^{'} \equiv x_1 - \bar{x}_1$, 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

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

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

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

$$\begin{bmatrix}\frac{dh_1^{'}}{dt}\\ \frac{dh_2^{'}}{dt}\end{bmatrix} = \begin{bmatrix} -\frac{C_{v1}\sqrt{\rho g}}{2A_1\sqrt{(\bar{h}_1-\bar{h}_2)}} & \frac{C_{v1}\sqrt{\rho g}}{2A_1\sqrt{(\bar{h}_1-\bar{h}_2)}}\\ \frac{C_{v1}\sqrt{\rho g}}{2A_2\sqrt{(\bar{h}_1-\bar{h}_2)}} & -\frac{C_{v1}\sqrt{\rho g}}{2A_2\sqrt{(\bar{h}_1-\bar{h}_2)}} - \frac{C_{v2}\sqrt{\rho g}}{2A_2\sqrt{\bar{h}_2}}\end{bmatrix}\begin{bmatrix}h_1^{'}\\ h_2^{'}\end{bmatrix} + \begin{bmatrix}\frac{1}{A_1}\\ 0\end{bmatrix} q_0^{'}$$

Laplace Transform – Main Idea

Linear ODEs

Example : 1st order ODE

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

$u(t)$ is a given time function.

"solve" involves integration. →

Solution

$$y(t) = \exp\left(-\frac{t}{\tau}\right) y(0) + \int_0^t \exp\left(-\frac{(t-\zeta)}{\tau}\right) u(\zeta)\, d\zeta$$

Table, Memorization

Laplace Transform ↓

Inverse Laplace Transform ↑

Partial Fraction E., Table, Memorization

$(\tau s + 1)\hat{y}(s) = \hat{u}(s)$

$\hat{u}(s)$ is a function of s, Laplace transform of u(t).

"solve" here involves just algebra! →

$$\hat{y}(s) = \frac{1}{(\tau s + 1)} \hat{u}(s)$$

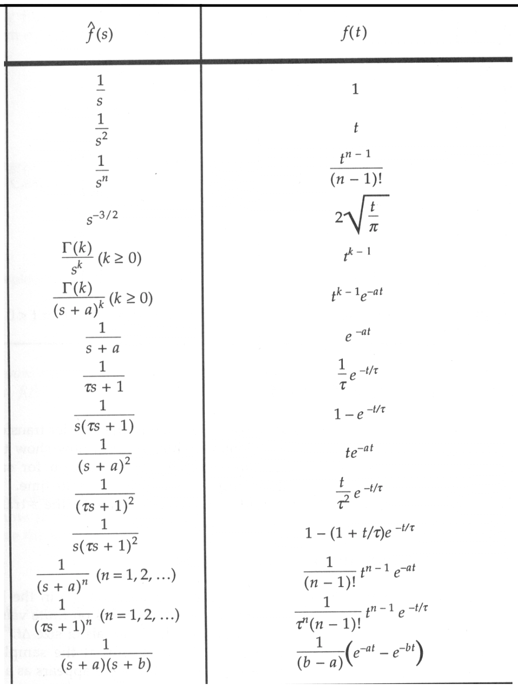
Laplace Transform – Key Points(1)

- Formula $\hat{f}(s) \equiv L\{f(t)\} \equiv \int_0^\infty f(t) e^{-st} dt \Rightarrow L^{-1}\{\hat{f}(s)\} = f(t)$
- Laplace Transform for simple signals
  - Steps, ramps, exponential decay or rise, pulse, impulse, etc.
  - Can be found by evaluating the integral.
  - See Table C2 of your textbook
  - Must memorize the simple ones.
- Important Properties

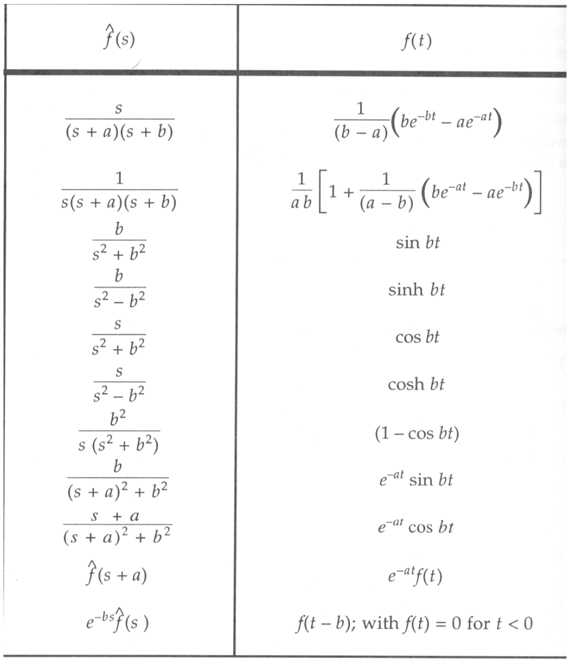
This is what enables us to convert linear ODEs into linear algebraic equations

$$L\left\{\frac{df}{dt}\right\} \equiv s \cdot \hat{f}(s) - f(0), \quad L\left\{\frac{d^2 f}{dt^2}\right\} \equiv s^2 \cdot \hat{f}(s) - s \cdot f(0) - f'(0), \text{ etc.}$$

$$L\left\{\int_0^t f(\zeta) d\zeta\right\} = \frac{1}{s} \hat{f}(s); \qquad L\{f(t-\delta)\} = \hat{f}(s) e^{-\delta s}$$



$\hat{f}(s)$	$f(t)$
$\frac{1}{s}$	1
$\frac{1}{s^2}$	t
$\frac{1}{s^n}$	$\frac{t^{n-1}}{(n-1)!}$
$s^{-3/2}$	$2\sqrt{\frac{t}{\pi}}$
$\frac{\Gamma(k)}{s^k}\ (k \geq 0)$	t^{k-1}
$\frac{\Gamma(k)}{(s+a)^k}\ (k \geq 0)$	$t^{k-1}e^{-at}$
$\frac{1}{s+a}$	e^{-at}
$\frac{1}{\tau s+1}$	$\frac{1}{\tau}e^{-t/\tau}$
$\frac{1}{s(\tau s+1)}$	$1-e^{-t/\tau}$
$\frac{1}{(s+a)^2}$	te^{-at}
$\frac{1}{(\tau s+1)^2}$	$\frac{t}{\tau^2}e^{-t/\tau}$
$\frac{1}{s(\tau s+1)^2}$	$1-(1+t/\tau)e^{-t/\tau}$
$\frac{1}{(s+a)^n}\ (n=1,2,\ldots)$	$\frac{1}{(n-1)!}t^{n-1}e^{-at}$
$\frac{1}{(\tau s+1)^n}\ (n=1,2,\ldots)$	$\frac{1}{\tau^n(n-1)!}t^{n-1}e^{-t/\tau}$
$\frac{1}{(s+a)(s+b)}$	$\frac{1}{(b-a)}\left(e^{-at}-e^{-bt}\right)$



$\hat{f}(s)$	$f(t)$
$\frac{s}{(s+a)(s+b)}$	$\frac{1}{(b-a)}\left(be^{-bt}-ae^{-at}\right)$
$\frac{1}{s(s+a)(s+b)}$	$\frac{1}{ab}\left[1+\frac{1}{(a-b)}\left(be^{-at}-ae^{-bt}\right)\right]$
$\frac{b}{s^2+b^2}$	$\sin bt$
$\frac{b}{s^2-b^2}$	$\sinh bt$
$\frac{s}{s^2+b^2}$	$\cos bt$
$\frac{s}{s^2-b^2}$	$\cosh bt$
$\frac{b^2}{s(s^2+b^2)}$	$(1-\cos bt)$
$\frac{b}{(s+a)^2+b^2}$	$e^{-at}\sin bt$
$\frac{s+a}{(s+a)^2+b^2}$	$e^{-at}\cos bt$
$\hat{f}(s+a)$	$e^{-at}f(t)$
$e^{-bs}\hat{f}(s)$	$f(t-b)$; with $f(t)=0$ for $t<0$

Laplace Transform – Key Points(2)

- Laplace Transform is a linear operation.

$$L\left\{a\cdot f_1(t)+b\cdot f_2(t)\right\}=a\cdot \hat{f}_1(s)+b\cdot \hat{f}_2(s)$$

- 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.
  - Final and Initial Value Theorem.

$$\lim_{t\to\infty} f(t)=\lim_{s\to 0} s\cdot \hat{f}(s); \qquad f(0)=\lim_{s\to\infty} s\cdot \hat{f}(s)$$

Laplace Transform – Key Points(3)

- Laplace transform does not work for solving nonlinear ODEs.

$$L\left\{y^2(t)\right\}\neq \hat{y}^2(s); L\left\{y(t)u(t)\right\}\neq \hat{y}(s)\cdot\hat{u}(s)$$

- See the supplementary note (posted on the class homepage) on Laplace transform for details.

Transfer Function

- Linear differential equation with a general forcing function (input)
  - 1st Order $a\frac{dy}{dt} + y(t) = ku(t)$
  - 2nd Order $b\frac{d^2y}{dt^2} + a\frac{dy}{dt} + y(t) = ku(t)$
  - Etc.
- 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 of zero) to arrive at a **general relationship between output and input.**

$$\hat{y}(s) = \frac{k}{(as+1)}\hat{u}(s)\,; \quad \hat{y}(s) = \frac{k}{(bs^2+as+1)}\hat{u}(s)$$

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

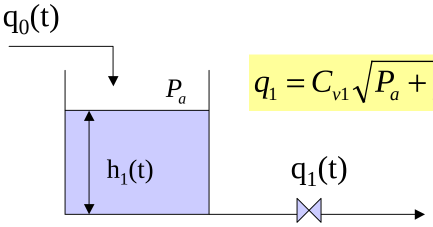
$$\hat{y}(s) = G(s)\cdot\hat{u}(s)$$

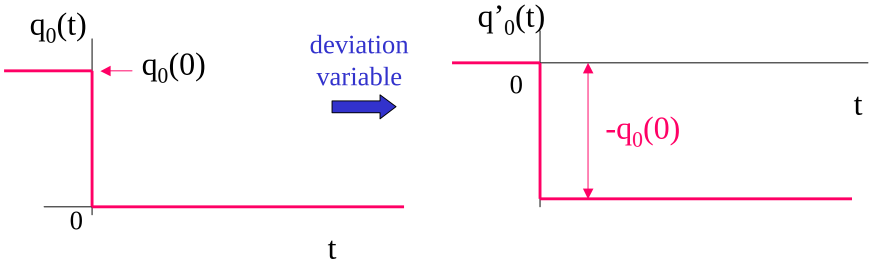
Example: Single-Tank Draining

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

$$\left(= \frac{\bar{q}_0^2}{C_{v1}^2 \rho g} \right)$$

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





Mass Balances

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

$$\Downarrow$$

$$A_1 \frac{dh_1}{dt} = q_0 - C_{v1}\sqrt{\rho g h_1}$$

Linearization (Linear Approximation)

$$A_1 \frac{dh_1}{dt} = q_0 - C_{v1}\sqrt{\rho g h_1}$$

$q_0^{'} \equiv q_0 - \bar{q}_0, h_1^{'} \equiv h_1 - \bar{h}_1, etc.$ $\Downarrow$ Linearize at the steady state of

$q_0 = \bar{q}_0, h_1 = \bar{h}_1$

$$A_1 \frac{dh_1^{'}}{dt} = q_0^{'} - \underbrace{\left(\frac{C_{v1}\sqrt{\rho g}}{2\sqrt{\bar{h}_1}}\right)}_{1/R_1} h_1^{'}$$

The above can be solved (using Laplace Transform) but will the linear model be valid throughout the entire draining experiment?

Solution Based on the Linearized Model

$$A_1 \frac{dh_1'}{dt} = q_0' - \frac{1}{R_1} h_1' \text{ with } h_1'(0) = 0 \text{ and } q_0'(s) = -\frac{\bar{q}_0}{s}$$

$$\Downarrow \; L$$

$$\left(A_1 s + \frac{1}{R_1}\right)\hat{h}_1'(\mathrm{s}) = -\frac{\bar{q}_0}{s} \Rightarrow \hat{h}_1'(\mathrm{s}) = \frac{-\bar{q}_0}{s\left(A_1 s + \frac{1}{R_1}\right)} = \frac{-\bar{q}_0 R_1}{s} + \frac{\bar{q}_0 R_1}{\left(s + \frac{1}{A_1 R_1}\right)}$$

$$\Downarrow \; L^{-1}$$

$$h_1'(t) = -\bar{q}_0 R_1\left(1 - \exp\left(-\frac{t}{A_1 R_1}\right)\right) \Rightarrow h_1(t) = \bar{h}_1 - \bar{q}_0 R_1\left(1 - \exp\left(-\frac{t}{A_1 R_1}\right)\right)$$

- 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

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

$$\frac{1}{\sqrt{h_1}} \frac{dh_1}{dt} = -\frac{C_{v1}\sqrt{\rho g}}{A_1},$$

$$\Downarrow$$

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

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

Laplace Transform of a 2x2 System

$$\begin{bmatrix}\dot{x}_1'\\ \dot{x}_2'\end{bmatrix} = A\begin{bmatrix}x_1'\\ x_2'\end{bmatrix} + B\begin{bmatrix}u_1'\\ u_2'\end{bmatrix}$$

⬇ Laplace Transform

$$\begin{bmatrix} s\hat{x}_1'(s)-x_1'(0)\\ s\hat{x}_2'(s)-x_2'(0)\end{bmatrix} = A\begin{bmatrix}\hat{x}_1'(s)\\ \hat{x}_2'(s)\end{bmatrix}+B\begin{bmatrix}\hat{u}_1'(s)\\ \hat{u}_2'(s)\end{bmatrix}$$

$$\left(\begin{bmatrix}s&0\\0&s\end{bmatrix}-A\right)\begin{bmatrix}\hat{x}_1'(s)\\ \hat{x}_2'(s)\end{bmatrix} = \begin{bmatrix}x_1'(0)\\ x_2'(0)\end{bmatrix}+B\begin{bmatrix}\hat{u}_1'(s)\\ \hat{u}_2'(s)\end{bmatrix}$$

$$\begin{bmatrix}\hat{x}_1'(s)\\ \hat{x}_2'(s)\end{bmatrix} = \underbrace{\left(\begin{bmatrix}s&0\\0&s\end{bmatrix}-A\right)^{-1}\begin{bmatrix}x_1'(0)\\ x_2'(0)\end{bmatrix}}_{\text{Effect of Non-Zero Initial Condition}} + \underbrace{\left(\begin{bmatrix}s&0\\0&s\end{bmatrix}-A\right)^{-1}B\begin{bmatrix}\hat{u}_1'(s)\\ \hat{u}_2'(s)\end{bmatrix}}_{\text{Effect of Forcing Function}}$$

Example – Interacting Tanks

$$\begin{bmatrix}\dfrac{dh_1'}{dt}\\ \dfrac{dh_2'}{dt}\end{bmatrix} = \begin{bmatrix}-\dfrac{1}{A_1R_1} & \dfrac{1}{A_1R_1}\\ \dfrac{1}{A_2R_1} & -\dfrac{1}{A_2}\left(\dfrac{1}{R_1}+\dfrac{1}{R_2}\right)\end{bmatrix}\begin{bmatrix}h_1'\\ h_2'\end{bmatrix}+\begin{bmatrix}\dfrac{1}{A_1}\\ 0\end{bmatrix}q_0'$$

⬇ Laplace Transform

$$\begin{bmatrix}\hat{h}_1'(s)\\ \hat{h}_2'(s)\end{bmatrix} = \underbrace{\begin{bmatrix}s+\dfrac{1}{A_1R_1} & -\dfrac{1}{A_1R_1}\\ -\dfrac{1}{A_2R_1} & s+\dfrac{1}{A_2}\left(\dfrac{1}{R_1}+\dfrac{1}{R_2}\right)\end{bmatrix}^{-1}\begin{bmatrix}h_1'(0)\\ h_2'(0)\end{bmatrix}}_{\text{Effect of Non-Zero Initial Condition}}$$

$$+\underbrace{\begin{bmatrix}s+\dfrac{1}{A_1R_1} & -\dfrac{1}{A_1R_1}\\ -\dfrac{1}{A_2R_1} & s+\dfrac{1}{A_2}\left(\dfrac{1}{R_1}+\dfrac{1}{R_2}\right)\end{bmatrix}^{-1}\begin{bmatrix}\dfrac{1}{A_1}\\ 0\end{bmatrix}\hat{q}_0'(s)}_{\text{Effect of Inlet Flowrate Change}}$$

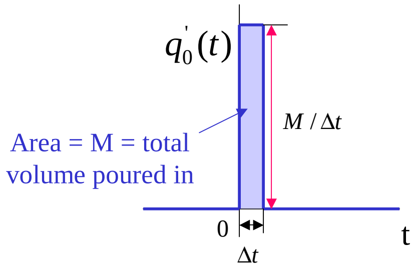
Example

- How will h_1 and h_2 respond in time if you "quickly" poured a beaker of water (M ml) into the first tank? Assume that you start at the equilibrium. ➡ $h_1'(0) = h_2'(0) = 0$

$$\begin{bmatrix}\hat{h}_1'(s)\\ \hat{h}_2'(s)\end{bmatrix} = \begin{bmatrix} \dfrac{\left(s+\frac{1}{A_2}\left(\frac{1}{R_1}+\frac{1}{R_2}\right)\right)\frac{1}{A_1}}{\left(s+\frac{1}{A_2}\left(\frac{1}{R_1}+\frac{1}{R_2}\right)\right)\left(s+\frac{1}{A_1R_1}\right)-\frac{1}{A_1A_2R_1^2}}\hat{q}_0'(s) \\[2em] \dfrac{\frac{1}{A_1A_2R_1}}{\left(s+\frac{1}{A_2}\left(\frac{1}{R_1}+\frac{1}{R_2}\right)\right)\left(s+\frac{1}{A_1R_1}\right)-\frac{1}{A_1A_2R_1^2}}\hat{q}_0'(s) \end{bmatrix}$$

Transfer Function

Example



$$\Delta t \to 0 \quad \Longrightarrow \quad \hat{q}_0'(s) = M$$

$$\begin{bmatrix}\hat{h}_1'(s)\\ \hat{h}_2'(s)\end{bmatrix} = \begin{bmatrix} \dfrac{\left(s+\frac{1}{A_2}\left(\frac{1}{R_1}+\frac{1}{R_2}\right)\right)\frac{M}{A_1}}{\left(s+\frac{1}{A_2}\left(\frac{1}{R_1}+\frac{1}{R_2}\right)\right)\left(s+\frac{1}{A_1R_1}\right)-\frac{1}{A_1A_2R_1^2}} \\[2em] \dfrac{\frac{M}{A_1A_2R_1}}{\left(s+\frac{1}{A_2}\left(\frac{1}{R_1}+\frac{1}{R_2}\right)\right)\left(s+\frac{1}{A_1R_1}\right)-\frac{1}{A_1A_2R_1^2}} \end{bmatrix}$$

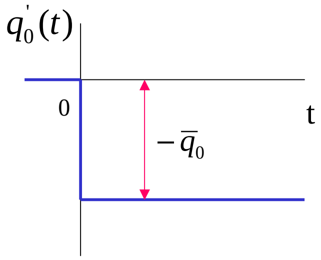
Inverse Laplace Transform ➡ $\begin{bmatrix}h_1'(t)\\ h_2'(t)\end{bmatrix}$

⬇

$$\begin{bmatrix}h_1(t)\\ h_2(t)\end{bmatrix} = \begin{bmatrix}h_1'(t)\\ h_2'(t)\end{bmatrix} + \begin{bmatrix}\bar{h}_1\\ \bar{h}_2\end{bmatrix}$$

Example

- How will h_1 and h_2 respond in time if you shut off the inlet flow at t=0? Assume that you start at the equilibrium. ⇨ $h_1^{'}(0) = h_2^{'}(0) = 0$



$$\xrightarrow{\quad} \quad \hat{q}_0^{'}(s) = \frac{-\bar{q}_0}{s}$$

Note for the lab: Since h gets far away from the steady-state value, the linearized model may become less and less valid as time increases. Use the nonlinear model directly in this case.

Example

$$\begin{bmatrix} \hat{h}_1^{'}(s) \\ \hat{h}_2^{'}(s) \end{bmatrix} = \begin{bmatrix} \dfrac{-\left(s + \dfrac{1}{A_2}\left(\dfrac{1}{R_1} + \dfrac{1}{R_2}\right)\right)\dfrac{\bar{q}_0}{A_1 s}}{\left(s + \dfrac{1}{A_2}\left(\dfrac{1}{R_1} + \dfrac{1}{R_2}\right)\right)\left(s + \dfrac{1}{A_1 R_1}\right) - \dfrac{1}{A_1 A_2 R_1^2}} \\ \dfrac{-\dfrac{1}{A_1 A_2 R_1}\dfrac{\bar{q}_0}{s}}{\left(s + \dfrac{1}{A_2}\left(\dfrac{1}{R_1} + \dfrac{1}{R_2}\right)\right)\left(s + \dfrac{1}{A_1 R_1}\right) - \dfrac{1}{A_1 A_2 R_1^2}} \end{bmatrix} \xrightarrow{\textit{Inverse Laplace Transform}} \begin{bmatrix} h_1^{'}(t) \\ h_2^{'}(t) \end{bmatrix}$$

$$\Downarrow$$

$$\begin{bmatrix} h_1(t) \\ h_2(t) \end{bmatrix} = \begin{bmatrix} h_1^{'}(t) \\ h_2^{'}(t) \end{bmatrix} + \begin{bmatrix} \bar{h}_1 \\ \bar{h}_2 \end{bmatrix}$$

Caution: The <u>Linearized Model</u> may not be valid for the entire duration of draining, as we mentioned earlier.

Example: Lab 5 (pH Experiment)

$$\begin{bmatrix} \dfrac{dC_A}{dt} \\ \dfrac{dC_B}{dt} \end{bmatrix} = \begin{bmatrix} F_A C_{Ai} - (F_A + F_B) C_A \\ F_B C_{Bi} - (F_A + F_B) C_B \end{bmatrix}$$

f: fraction of acid that reacted with base to produce water

$$pH = -\log_{10}[C_A(1-f)]$$

$$f = \frac{C_A + C_B}{2C_A} - \frac{\sqrt{(C_A - C_B) + 4 \cdot 10^{-14}}}{2C_A} \quad \Leftarrow [C_B - f \cdot C_A][C_A - f \cdot C_A] = 10^{-14}$$

Linearization w.r.t. $\overline{C}_A, \overline{C}_B, \overline{F}_A, \overline{F}_B$ should give

$$\begin{bmatrix} \dfrac{dC_A^{'}}{dt} \\ \dfrac{dC_B^{'}}{dt} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} C_A^{'} \\ C_B^{'} \end{bmatrix} + \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix} \begin{bmatrix} F_A^{'} \\ F_B^{'} \end{bmatrix}$$

$$pH^{'} = [c_1 \quad c_2] \begin{bmatrix} C_A^{'} \\ C_B^{'} \end{bmatrix}$$

Q: Where are the nonlinearities in the equations?

Generalization (n x n System)

Matrix Differential Equation

$$\dot{x}^{'} = A\,x^{'} + B\,u^{'}$$

$$y^{'} = Cx^{'} + D\,u^{'}$$

$$y^{'}(t) = Cx^{'}(t) + D\,u^{'}(t)$$

y is a particular linear combination of x and u that you want to calculate.

$$L \Big\downarrow \quad \Big\uparrow L^{-1}$$

$$\hat{x}^{'}(s) = (sI - A)^{-1} B\hat{u}^{'}(s)$$

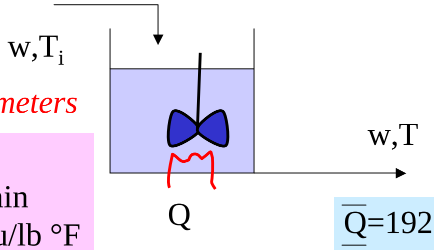
$$\hat{y}^{'}(s) = \underbrace{\big(C(sI - A)^{-1} B + D\big)}_{G(s)} \hat{u}^{'}(s)$$

Transfer function between u and y

Which one would you rather use for calculating x and y for given u?

Sample Test Problem 1

(Solutions are in the supplementary notes)



constant parameters

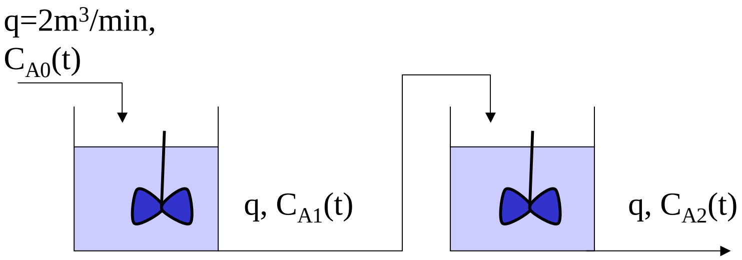
$V = 1.60\ ft^3$
$w = 200$ lb/min
$C_p = 0.32$ Btu/lb °F
$\rho = 62.4\ lb/ft^3$

steady-state values

$\bar{Q} = 1920$ Btu/min
$\bar{T}_i = 70$ °F

Suppose that T_i increased from 70 °F to 90 °F and Q dropped from 1920 Btu/min to 1600 Btu/min at t=0. Calculate the transient response of T. Assume that the tank was at the steady state at t=0.

Sample Test Problem 2



A→B
$r_1 = 0.5 C_{A1}(t)$ /min
$V_1 = 4 m^3$

A→B
$r_2 = 0.5 C_{A2}(t)$ /min
$V_2 = 3 m^3$

At steady state, $C_{A0} = \bar{C}_{A0} = 1 kgmol/m^3$

At t=0, engineer poured 2.5 kgmols of pure A into the first tank. Calculate the response of $C_{A1}(t)$ and $C_{A2}(t)$. Assume that the reactors were at their steady state at t=0.