Lecture Notes on
Mathematical Modeling of Chemical Processes

General Modeling Principles

1. The model equations are at best an approximation to the real process.
2. Modeling inherently involves a compromise between model accuracy and complexity on one hand, and the cost and effort required to develop the model, on the other hand.
3. Process modeling is both an art and a science. Creativity is required to make simplifying assumptions that result in an appropriate model.
4. Dynamic models of chemical processes consist of ordinary differential equations (ODE) and/or partial differential equations (PDE), plus related algebraic equations.

Physical Modeling Approaches

1. Thermodynamics, chemical kinetics (physical/chemical fundamental, global)
2. Model structure by theoretical analysis
3. Conservation Laws (Theoretical models of chemical processes are based on conservation laws.)
4. Heat, mass, and momentum transfer
5. Physical property relationships (viscosity, thermal conductivity, diffusivity)
6. Model complexity must be determined (assumptions, e. g. ideal gas)

Comment:

Can be computationally expensive (therefore, not real-time)
May be expensive/time-consuming to obtain
Good for extrapolation, scale-up
Does not require experimental data to obtain (data required for validation and fitting)

A Systematic Approach for Developing Dynamic Models

1. State the modeling objectives and the end use of the model. They determine the required levels of model detail and model accuracy.
2. Draw a schematic diagram of the process and label all process variables.
3. List all of the assumptions that are involved in developing the model. Try for parsimony; the model should be no more complicated than necessary to meet the modeling objectives.
4. Determine whether spatial variations of process variables are important. If so, a partial differential equation model will be required.
5. Write appropriate conservation equations (mass, component, energy, and so forth).

6. Introduce equilibrium relations and other algebraic equations (from thermodynamics, transport phenomena, chemical kinetics, equipment geometry, etc.).
7. Perform a degrees of freedom analysis to ensure that the model equations can be solved.
8. Simplify the model. It is often possible to arrange the equations so that the dependent variables (outputs) appear on the left side and the independent variables (inputs) appear on the right side. This model form is convenient for computer simulation and subsequent analysis.
9. Classify inputs as disturbance variables or as manipulated variables.

Empirical (Black box)

- Large number of unknown parameters
- Can be obtained quickly (e.g., linear regression)
- Model structure is subjective
- Dangerous to extrapolate

Semi-empirical

- Compromise of first two approaches
- Model structure may be simpler
- Typically 2 to 10 physical parameters estimated
    (nonlinear regression)
- Good versatility, can be extrapolated
- Can be run in real-time
- linear regression
- nonlinear regression
- number of parameters affects accuracy of model, but confidence limits on the parameters fitted must be evaluated
- objective function for data fitting – minimize sum of squares of errors between data points and model predictions (use optimization code to fit parameters)
- nonlinear models such as neural nets are becoming popular (automatic modeling)

Uses of Mathematical Modeling

- to improve understanding of the process
- to optimize process design/operating conditions
- to design a control strategy for the process
- to train operating personnel

Conservation of Mass

$$
\left\{ \begin{array}{c} \text{rate of mass} \\ \text{accumulation} \end{array} \right\} = \left\{ \begin{array}{c} \text{rate of mass} \\ \text{in} \end{array} \right\} - \left\{ \begin{array}{c} \text{rate of mass} \\ \text{out} \end{array} \right\}
$$

Conservation of Component *i*

$$
\left\{ \begin{array}{c} \text{rate of component i} \\ \text{accumulation} \end{array} \right\} = \left\{ \begin{array}{c} \text{rate of component i} \\ \text{in} \end{array} \right\}
$$
$$
- \left\{ \begin{array}{c} \text{rate of component i} \\ \text{out} \end{array} \right\} + \left\{ \begin{array}{c} \text{rate of component i} \\ \text{produced} \end{array} \right\}
$$

Conservation of Energy

The general law of energy conservation is also called the First Law of Thermodynamics. It can be expressed as:

$$
\left\{ \begin{array}{c} \text{rate of energy} \\ \text{accumulation} \end{array} \right\} = \left\{ \begin{array}{c} \text{rate of energy in} \\ \text{by convection} \end{array} \right\} - \left\{ \begin{array}{c} \text{rate of energy out} \\ \text{by convection} \end{array} \right\}
$$
$$
+ \left\{ \begin{array}{c} \text{net rate of heat addition} \\ \text{to the system from} \\ \text{the surroundings} \end{array} \right\} + \left\{ \begin{array}{c} \text{net rate of work} \\ \text{performed on the system} \\ \text{by the surroundings} \end{array} \right\}
$$

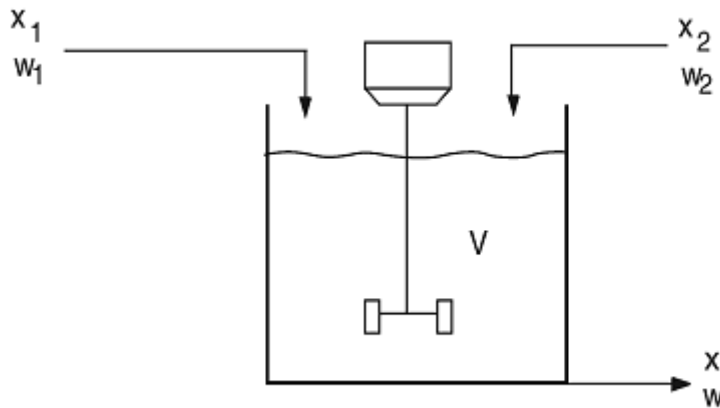**Example 1: A Blending Process (discussed in Lecture I)**

Figure 1. Stirred-tank blending process

An unsteady-state mass balance for the blending system:

$$\left\{ \begin{array}{c} \text{rate of mass} \\ \text{accumulation} \end{array} \right\} = \left\{ \begin{array}{c} \text{rate of mass} \\ \text{in} \end{array} \right\} - \left\{ \begin{array}{c} \text{rate of mass} \\ \text{out} \end{array} \right\}$$

that is

$$\frac{d(V\rho)}{dt} = w_1 + w_2 - w \qquad\qquad 1$$

where w_1, w_2, and w are mass flow rates.

The unsteady-state component balance is:

$$\left\{ \begin{array}{c} \text{rate of component i} \\ \text{accumulation} \end{array} \right\} = \left\{ \begin{array}{c} \text{rate of component i} \\ \text{in} \end{array} \right\}$$

$$- \left\{ \begin{array}{c} \text{rate of component i} \\ \text{out} \end{array} \right\} + \left\{ \begin{array}{c} \text{rate of component i} \\ \text{produced} \end{array} \right\}$$

that is

$$\frac{d(V\rho x)}{dt} = w_1 x_1 + w_2 x_2 - wx \qquad\qquad 2$$

The corresponding steady-state model was derived in Lecture I:

$$0 = \overline{w}_1 + \overline{w}_2 - \overline{w} \qquad\qquad 3$$

$$0 = \overline{w}_1 \overline{x}_1 + \overline{w}_2 \overline{x}_2 - \overline{w}\overline{x} \qquad\qquad 4$$

For constant ρ, Eqs. 1 and 2 become:

$$\rho \frac{dV}{dt} = w_1 + w_2 - w \qquad\qquad 5$$

$$\rho \frac{d(Vx)}{dt} = w_1 x_1 + w_2 x_2 - wx \qquad\qquad 6$$

Equation 6 can be simplified by expanding the accumulation term (left side) using the "chain rule" for differentiation of a product:

$$\rho \frac{d(Vx)}{dt} = \rho V \frac{d(x)}{dt} + \rho x \frac{d(V)}{dt} \qquad\qquad 7$$

Substitution of 7 into 6 gives:

$$\rho V \frac{d(x)}{dt} + \rho x \frac{d(V)}{dt} = w_1 x_1 + w_2 x_2 - wx \qquad 8$$

Substitution of the mass balance in 5 for $\rho dV / dt$ in 8 gives:

$$\rho V \frac{d(x)}{dt} + x(w_1 + w_2 - w) = w_1 x_1 + w_2 x_2 - wx \qquad 9$$

After canceling common terms and rearranging 5 and 9, a more convenient model form is obtained:

$$\frac{dV}{dt} = \frac{1}{\rho}(w_1 + w_2 - w) \qquad 10$$

$$\frac{dx}{dt} = \frac{w_1}{V\rho}(x_1 - x) + \frac{w_2}{V\rho}(x_2 - x) \qquad 11$$

Rearrange Eq.6,

$$\rho V \frac{dx}{dt} + wx = w_1 x_1 + w_2 x_2 \qquad 12$$

At steady state, Eq.6 becomes,

$$w^0 x^0 = w_1^0 x_1^0 + w_2^0 x_2^0 \qquad 13$$

$$\rho V \frac{d(x^0 + \Delta x)}{dt} + w(x^0 + \Delta x) = x_1^0(w_1^0 + \Delta w_1) + w_2^0 x_2^0 \qquad 14$$

Subtract Eq.13 from Eq.14,

$$\rho V \frac{d(\Delta x)}{dt} + w(\Delta x) = x_1^0(\Delta w_1) \qquad 15$$

Similarly,

$$\rho V \frac{d(\Delta x)}{dt} + w(\Delta x) = x_2^0(\Delta w_2) \qquad 16$$

$$\rho V \frac{d(\Delta x)}{dt} + w(\Delta x) = w_1^0(\Delta x_1) \qquad 17$$

Let $x = \Delta x$, $w_1 = \Delta w_1$, $w_2 = \Delta w_2$ and $x_1 = \Delta x_1$,

$$\rho V \frac{dx}{dt} + wx = x_1^0 w_1 \qquad\qquad 18$$

$$\rho V \frac{dx}{dt} + wx = x_2^0 w_2 \qquad\qquad 19$$

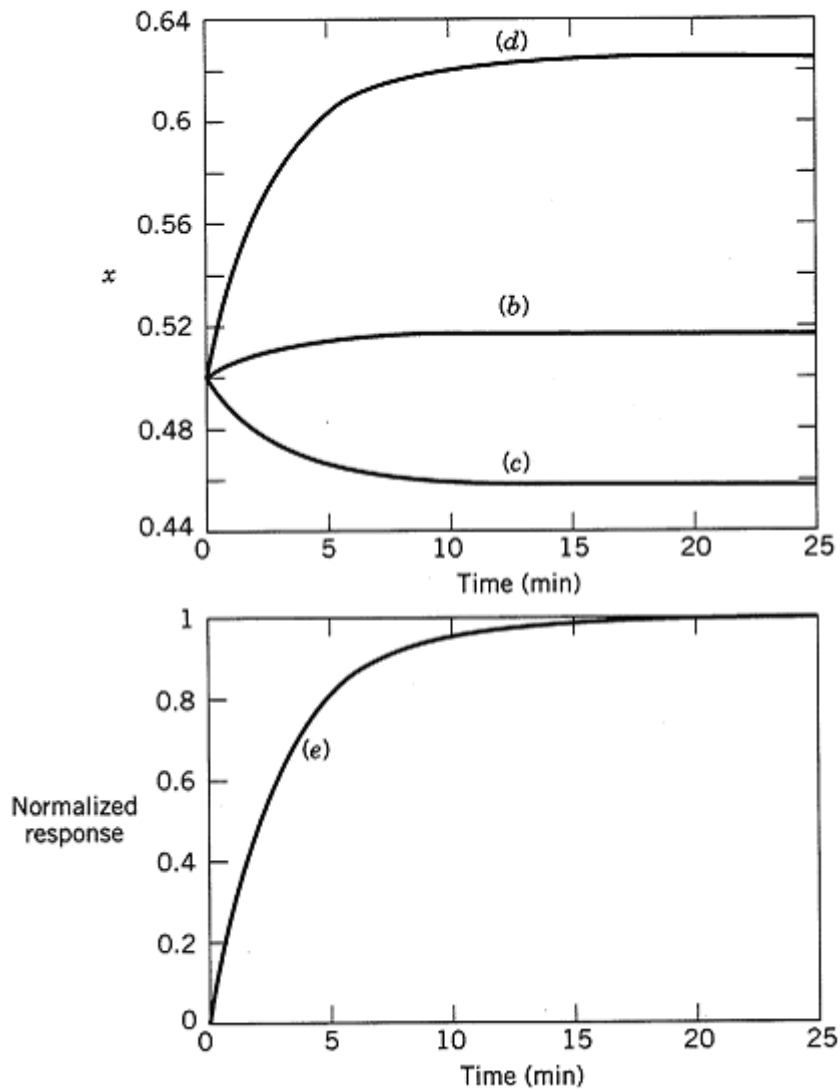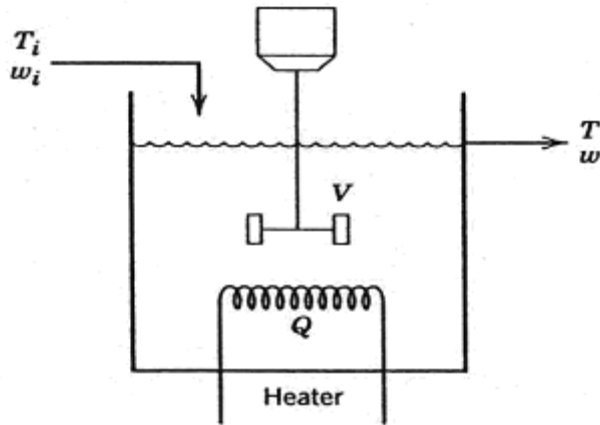$$\rho V \frac{dx}{dt} + wx = w_1^0 x_1 \qquad\qquad 20$$

Figure 2. Exit composition responses of a stirred-tank blending process to step changes in:
- (b) flow rate w_1
- (c) flow rate w_2
- (d) inlet composition x_1

(e) Normalized response for parts (b)-(d).

Example 2: Stirred-Tank Heating Process with constant holdup, V

Assumptions:

1. Perfect mixing; thus, the exit temperature T is also the temperature of the tank contents.
2. The liquid holdup V is constant because the inlet and outlet flow rates are equal.
3. The density and heat capacity C of the liquid are assumed to be constant. Thus, their temperature dependence is neglected.
4. Heat losses are negligible.

In addition, for the processes and examples considered in this course, it is appropriate to make two assumptions:

1. Changes in potential energy and kinetic energy can be neglected because they are small in comparison with changes in internal energy.
2. The net rate of work can be neglected because it is small compared to the rates of heat transfer and convection.

For these reasonable assumptions, the energy balance

$$
\begin{Bmatrix} \text{rate of energy} \\ \text{accumulation} \end{Bmatrix} = \begin{Bmatrix} \text{rate of energy in} \\ \text{by convection} \end{Bmatrix} - \begin{Bmatrix} \text{rate of energy out} \\ \text{by convection} \end{Bmatrix}
$$

$$
+ \begin{Bmatrix} \text{net rate of heat addition} \\ \text{to the system from} \\ \text{the surroundings} \end{Bmatrix} + \begin{Bmatrix} \text{net rate of work} \\ \text{performed on the system} \\ \text{by the surroundings} \end{Bmatrix}
$$

that is

$$\frac{dU_{int}}{dt} = -\Delta(w\hat{H}) + Q \qquad\qquad 21$$

where

        U_{int} = the internal energy of the system

        $\hat{H}$ = enthalpy per unit mass

        w = mass flow rate

        Q = rate of heat transfer to the system

        Δ = denotes the difference between outlet and inlet conditions of the flowing streams; therefore

  $-\Delta(w\hat{H})$ = rate of enthalpy of the inlet stream(s)-the enthalpy of the outlet stream(s)

Model Development

The definition of the enthalpy of a pure substance,

$$H = U_{int} + pV \qquad\qquad 22$$

Therefore, for a pure liquid at low or moderate pressures, the internal energy is approximately equal to the enthalpy, $U_{int} \approx H$, and H depends only on temperature. From the laws of thermodynamics, a differential change in temperature, dT, produces a corresponding change in the internal energy per unit mass, $d\hat{U}_{int}$,

$$d\hat{U}_{int} = d\hat{H} = CdT \qquad\qquad 23$$

where C is the constant pressure heat capacity (assumed to be constant). The total internal energy of the liquid in the tank is:

$$U_{int} = \rho V \hat{U}_{int} \qquad\qquad 24$$

An expression for the rate of internal energy accumulation can be derived from Eqs.14 and 15:

$$\frac{dU_{int}}{dt} = \rho VC \frac{dT}{dt} \qquad\qquad 25$$

Note that this term appears in the general energy balance of Eq.21.

Suppose that the liquid in the tank is at a temperature T and has an enthalpy, $\hat{H}$. Integrating Eq.14 from a reference temperature T_{ref} to T gives,

$$\hat{H} - \hat{H}_{ref} = C(T - T_{ref}) \qquad\qquad 26$$

where $\hat{H}_{ref}$ is the value of $\hat{H}$ at T_{ref}. Without loss of generality, we assume that $\hat{H}_{ref} = 0$. Thus, Eq.26 can be written as:

$$\hat{H} = C(T - T_{ref}) \qquad\qquad 27$$

For the inlet stream

$$\hat{H}_i = C(T_i - T_{ref}) \qquad\qquad 28$$

Substituting Eq.27 and 28 into the convection term of Eq.26 gives:

$$-\Delta(wH) = w\left[C(T_i - T_{ref})\right] - w\left[C(T - T_{ref})\right] \qquad\qquad 29$$

Finally, substitution of Eq.25 and 29 into 21

$$\rho V C \frac{dT}{dt} = wC(T_i - T) + Q \qquad\qquad 30$$

Rearrange Eq.30,

$$\rho V C \frac{dT_{out}}{dt} + w_{in} C T_{out} = w_{in} C T_{in} + Q_{in} \qquad\qquad 31$$

At steady state,

$$wCT_{out}^0 = w_{in} C T_{in}^0 + Q_{in}^0 \qquad\qquad 32$$

Let

$$T_{out} = T_{out}^0 + \Delta T_{out}$$
$$T_{in} = T_{in}^0 \qquad\qquad 33$$
$$Q_{in} = Q_{in}^0 + \Delta Q_{in}$$

$$\rho V C \frac{d(T_{out}^0 + \Delta T_{out})}{dt} + w_{in} C(T_{out}^0 + \Delta T_{out}) = w_{in} C T_{in} + Q_{in}^0 + \Delta Q_{in} \qquad 34$$

Subtract Eq.32 from Eq.34

$$\rho V C \frac{d\Delta T_{out}}{dt} + w_{in} C\Delta T_{out} = \Delta Q_{in} \qquad\qquad 35$$

Let

$$T_{out} = T_{out}^0 + \Delta T_{out}$$

$$T_{in} = T_{in}^0 + \Delta T_{in} \qquad 36$$

$$Q_{in} = Q_{in}^0$$

$$\rho VC \frac{d(T_{out}^0 + \Delta T_{out})}{dt} + w_{in} C(T_{out}^0 + \Delta T_{out}) = w_{in} C(T_{in}^0 + \Delta T_{in}) + Q_{in}^0 \qquad 37$$

Subtract Eq.232 from Eq.37

$$\rho VC \frac{d\Delta T_{out}}{dt} + w_{in} C \Delta T_{out} = w_{in} C \Delta T_{in} \qquad 38$$

Rearrange Eqs.35 and 38

$$\frac{\rho V}{w_{in}} \frac{d\Delta T_{out}}{dt} + \Delta T_{out} = \frac{1}{w_{in}} \Delta Q_{in} \qquad 39$$

$$\frac{\rho V}{w_{in}} \frac{d\Delta T_{out}}{dt} + \Delta T_{out} = \Delta T_{in} \qquad 40$$
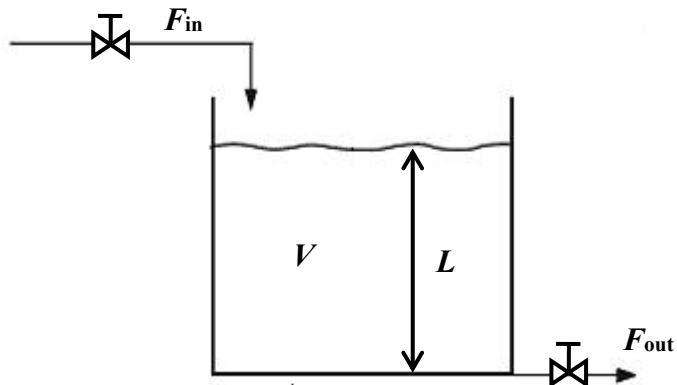
Example 3 Surge Tank

Figure 4. Surge Tank

Mass balance (assume constant density),

$$\frac{dV}{dt} = F_{in} - F_{out} \qquad 41$$

Use the knowledge you learned from the Unit Operation of Chemical Engineering, in the laminar flow region,

$$F_{out} = C_v' L \qquad\qquad 42$$

where C_v' is the flow parameter
also,

$$\frac{dV}{dt} = A\frac{dL}{dt} \qquad\qquad 43$$

where A is the cross section of the tank.
therefore,

$$A\frac{dL}{dt} + C_v' L = F_{in}. \qquad\qquad 44$$

From mass balance,

$$F_{in} = F_{out} \qquad\qquad 45$$

At steady state,

$$F_{in}^0 = F_{out}^0 = C_v' L^0 \qquad\qquad 46$$

$$A\frac{d(L^0 + \Delta L)}{dt} + C_v'(L^0 + \Delta L) = (F_{in}^0 + \Delta F_{in}) \qquad\qquad 47$$

$$A\frac{d\Delta L}{dt} + C_v'\Delta L = \Delta F_{in} \qquad\qquad 48$$

Rearrange,

$$\frac{A}{C_v'}\frac{d\Delta L}{dt} + \Delta L = \frac{1}{C_v'}\Delta F_{in} \qquad\qquad 49$$

Similarly,

$$\frac{A}{C_v'}\frac{d\Delta L}{dt} + \Delta L = \frac{-1}{C_v'}\Delta F_{out} \qquad\qquad 50$$

Combine

$$\frac{A}{C_v'}\frac{d\Delta L}{dt} + \Delta L = \frac{1}{C_v'}(\Delta F_{in} - \Delta F_{out}) \qquad\qquad 51$$

When flow is large, it becomes turbulent, then,

$$F_{out} = C_v \sqrt{L}$$ 52

Let K be the slope of the tangent of the *F-L* curve at the set point,

$$K = \left. \frac{dF_{out}}{dL} \right|_{L=L^0} = \left. \frac{d(C_v \sqrt{L})}{dL} \right|_{L=L^0} = \frac{C_v}{2\sqrt{L^0}}$$ 53

therefore,

$$\Delta F_{out} = \frac{C_v}{2\sqrt{L^0}} \Delta L$$ 54

$$\begin{aligned} F_{out} &= F_{out}^0 + \Delta F_{out} \\ &= F_{out}^0 + \frac{C_v}{2\sqrt{L^0}} \Delta L \end{aligned}$$ 55

Substitute back to the mass balance equation,

$$\frac{dV}{dt} = A\frac{dL}{dt} = F_{in} - F_{out}^0 - \frac{C_v}{2\sqrt{L^0}} \Delta L$$ 56

and

$$A\frac{d(L^0 + \Delta L)}{dt} = (F_{in}^0 + \Delta F_{in}) - F_{out}^0 - \frac{C_v}{2\sqrt{L^0}} \Delta L$$ 57

therefore

$$A\frac{d\Delta L}{dt} = \Delta F_{in} - \frac{C_v}{2\sqrt{L^0}} \Delta L$$ 58

After rearrange,

$$\frac{A}{C_v \Big/ 2\sqrt{L^0}} \frac{d\Delta L}{dt} + \Delta L = \frac{1}{C_v \Big/ 2\sqrt{L^0}} \Delta F_{in}$$ 59

General form of the first order system

Let $y = T_{out}$ and $x = T_{in}$, omit Δ for simplicity,

$$\tau \frac{dy}{dt} + y = Kx$$ 60

where τ is called the time constant, K is the gain, y is the output variable, and x is the input variable.

Time constant τ = Resister R × Capacity C

Heat Resister $R = \dfrac{\Delta T}{q} = \dfrac{1}{F_{in}C} = \dfrac{\Delta T}{F_{in}\Delta U}$

Flow Resister $R = \dfrac{\Delta L}{F_{out}} = \dfrac{2\sqrt{L_0}}{C_v}$

Heat Capacity $C = \dfrac{\Delta U}{\Delta T_{out}}$

Flow Capacity $C = \dfrac{\Delta V}{\Delta L}$

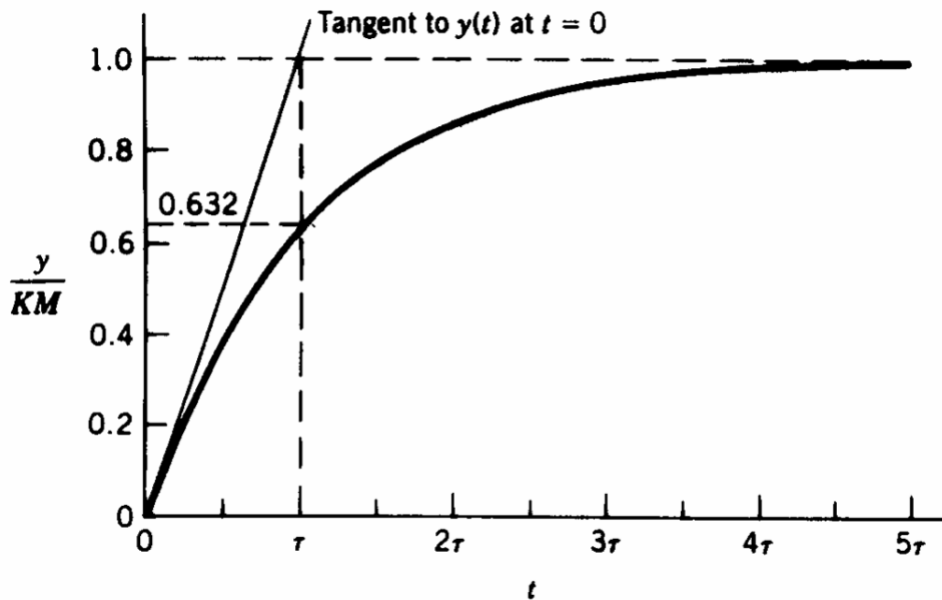Let $x = u = 1$ (step input), $y(t) = K\left(1 - e^{-\frac{t}{\tau}}\right)_{t=\tau} = 0.632$.
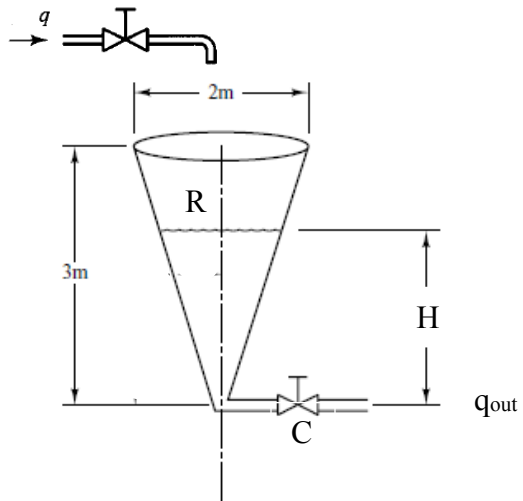

Figure 5. Step response of a first order system

Mathematical Modeling of Chemical Processes I
ChE@TongjiU, Min Huang, PhD, 2022

Quiz VI

Find the mathematical model of the following configuration

$$V = \frac{1}{3}\pi r^2 h$$

$$r = \frac{1}{3}h$$

$$V = \frac{1}{3}\pi \left(\frac{h}{3}\right)^2 h = \frac{1}{27}\pi h^3$$

$$\rho dV = \rho \left(\frac{1}{9}\pi h^2 dh\right) = q_{out} - q_{in}$$
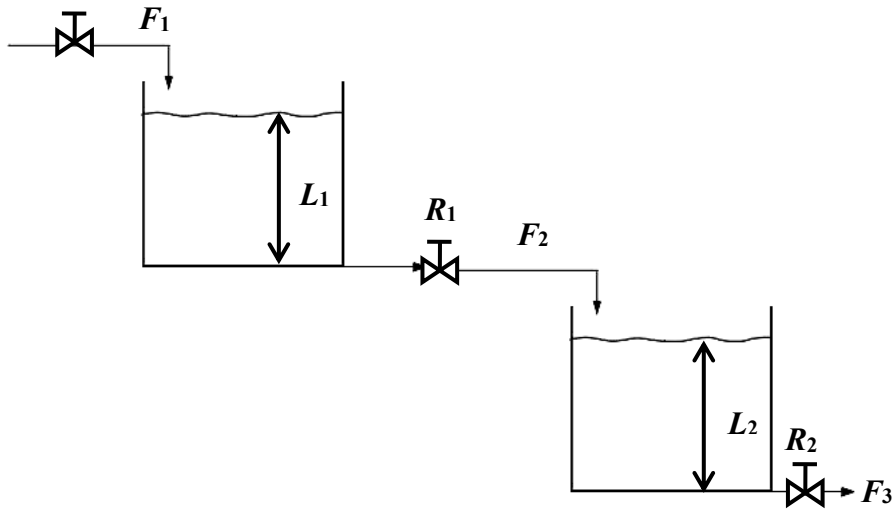
$$q = Cv\sqrt{h}$$

Example 5. Tanks in series

Figure 6. Tanks in series

Mass balance,

$$A_1 \frac{dL_1}{dt} = F_1 - F_2 \qquad \qquad 73$$

$$F_2 = \frac{L_1}{R_1} \qquad \qquad 74$$

$$A_2 \frac{dL_2}{dt} = F_2 - F_3 \qquad \qquad 75$$

$$F_3 = \frac{L_2}{R_2} \qquad \qquad 76$$

where A_1, A_2 are the capacity of tank 1 and tank 2,
R_1, R_2 are the resister of tank 1 and tank 2,
assume they are all linear.

$$A_1 \frac{dL_1}{dt} + \frac{L_1}{R_1} = F_1 \qquad \qquad 77$$

$$A_2 \frac{dL_2}{dt} + \frac{L_2}{R_2} = \frac{L_1}{R_1} \qquad \qquad 78$$

$$L_1 = R_1 A_2 \frac{dL_2}{dt} + \frac{R_1}{R_2} L_2 \qquad \qquad 79$$

differentiate

$$\frac{dL_1}{dt} = R_1 A_2 \frac{d^2 L_2}{dt^2} + \frac{R_1}{R_2} \frac{dL_2}{dt} \qquad 80$$

$$A_1 R_1 A_2 R_2 \frac{d^2 L_2}{dt^2} + (A_1 R_1 + A_2 R_2) \frac{dL_2}{dt} + L_2 = R_2 F_1 \qquad 81$$

let $T_1 = A_1 R_1$ and $T_2 = A_2 R_2$,

$$T_1 T_2 \frac{d^2 L_2}{dt^2} + (T_1 + T_2) \frac{dL_2}{dt} + L_2 = R_2 F_1 \qquad 82$$

This is a second order system.

$$\underline{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} L_2 \\ \dot{L}_2 \end{bmatrix}$$

$$\underline{\dot{x}} = \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} 0 L_2 + \dot{L}_2 \\ -\dfrac{1}{T_1 T_2} L_2 - \dfrac{T_1 + T_2}{T_1 T_2} \dot{L}_2 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & \dfrac{R_2 F_1}{T_1 T_2} \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 1 \\ -\dfrac{1}{T_1 T_2} & -\dfrac{T_1 + T_2}{T_1 T_2} \end{bmatrix} \begin{bmatrix} L_2 \\ \dot{L}_2 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & \dfrac{R_2}{T_1 T_2} \end{bmatrix} \begin{bmatrix} 0 \\ F_1 \end{bmatrix}$$

$$\underline{\underline{P}} = \begin{bmatrix} 0 & 1 \\ -\dfrac{1}{T_1 T_2} & -\dfrac{T_1 + T_2}{T_1 T_2} \end{bmatrix}$$

$$\underline{\underline{B}} = \begin{bmatrix} 0 & 0 \\ 0 & \dfrac{R_2}{T_1 T_2} \end{bmatrix}$$

$$\underline{c} = \underline{\underline{L}}\, \underline{x}$$

$$\underline{c} = \begin{bmatrix} L_2 \end{bmatrix}$$

$$\underline{\underline{L}} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\underline{c} = \begin{bmatrix} \\ c \end{bmatrix} = \begin{bmatrix} L_2 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

What about L_1 ?
in surge tank cases, liquid level/ holdup is what we care the most

Example 4. Modeling Surge Tank + Blending Using State Space Techniques

Recall Eqs.5, 6 and 52 assume constant density,

$$\frac{dV}{dt} = F_1(t) + F_2(t) - F(t) \qquad\qquad 5$$

$$\frac{d(V(t)x(t))}{dt} = F_1(t)x_1(t) + F_2(t)x_2(t) - F(t)x(t) \qquad\qquad 6$$

$$F(t) = C_v\sqrt{L(t)} = C_v\sqrt{L(t)} \qquad\qquad 52$$

At steady state,

$$F_1^0(t) + F_2^0(t) - F^0(t) = 0 \qquad\qquad 63$$

$$F_1^0(t)x_1(t) + F_2^0(t)x_2(t) - F(t)^0 x(t) = 0 \qquad\qquad 64$$

$$F^0(t) = C_v\sqrt{\frac{V^0}{A}} \qquad\qquad 65$$

Assume small deviations about this point, let,

$$F_1(t) = F_1^0 + \mu_1(t) \qquad\qquad \text{in} \qquad\qquad 66$$

$$F_2(t) = F_2^0 + \mu_2(t) \qquad\qquad \text{in} \qquad\qquad 67$$

$$V(t) = V^0 + \xi_1(t) \qquad\qquad \text{out} \qquad\qquad 68$$

$$x(t) = x^0 + \xi_2(t) \qquad\qquad \text{out} \qquad\qquad 69$$

Also recall the linearization procedure

$$K = \left.\frac{dF}{dL}\right|_{L=L^0} = \left.\frac{d(C_v\sqrt{L})}{dL}\right|_{L=L^0} = \frac{C_v}{2\sqrt{L^0}} \qquad\qquad 53$$

Similarly,

$$K = \left.\frac{dF}{dV}\right|_{V=V^0} = \left.\frac{d(C_v\sqrt{V/A})}{dV}\right|_{V=V^0} = \frac{C_v}{2\sqrt{AV^0}} \qquad\qquad 70$$

$$\Delta F = \frac{C_v}{2\sqrt{AV^0}}\Delta V = \frac{C_v}{2\sqrt{AV^0}}\xi_1(t) \qquad\qquad 71$$

$$\frac{F^0}{V^0} = \frac{C_V\sqrt{\dfrac{V^0}{A}}}{V^0} = \frac{C_v}{\sqrt{AV^0}} \qquad\qquad 72$$

$$V(t) = V^0 + \xi_1(t) \qquad\qquad\qquad \text{out} \qquad\qquad 68$$

$$F = F^0 + \frac{1}{2}\frac{F^0}{V^0}\xi_1(t) \qquad\qquad 73$$

Substitute Eqs.66, 67, 68, 69 and 73 back to Eqs.5 and 6 and subtract Eqs.63 and 64,

$$\frac{dV}{dt} = F_1(t) + F_2(t) - F(t) \qquad\qquad 5$$

$$\frac{d(V(t)x(t))}{dt} = F_1(t)x_1(t) + F_2(t)x_2(t) - F(t)x(t) \qquad\qquad 6$$

$$F_1^0(t) + F_2^0(t) - F^0(t) = 0 \qquad\qquad 63$$

$$F_1^0(t)x_1(t) + F_2^0(t)x_2(t) - F(t)^0 x(t) = 0 \qquad\qquad 64$$

$$F_1(t) = F_1^0 + \mu_1(t) \qquad\qquad 66$$

$$F_2(t) = F_2^0 + \mu_2(t) \qquad\qquad 67$$

$$V(t) = V^0 + \xi_1(t) \qquad\qquad 68$$

$$x(t) = x^0 + \xi_2(t) \qquad\qquad 69$$

$$F = F^0 + \frac{1}{2}\frac{F^0}{V^0}\xi_1(t) \qquad\qquad 73$$

Equation 5 becomes

$$\frac{dV}{dt} = F_1^0 + \mu_1 + F_2^0 + \mu_2 - F^0 - \frac{1}{2}\frac{F^0}{V^0}\xi_1$$

Subtract 63

$$\frac{dV}{dt} = \frac{d(V^0 + \xi_1(t))}{dt}$$

$$= \frac{d\xi_1}{dt} = \mu_1 + \mu_2 - \frac{1}{2}\frac{F^0}{V^0}\xi_1 \qquad\qquad 70$$

Equation 6 becomes

$$x^0\frac{dV}{dt} + V^0\frac{dx}{dt} = (F_1^0 + \mu_1)x_1 + (F_2^0 + \mu_2)x_2 - F^0(x^0 + \xi_2)$$

Subtract 64

$$V^0\frac{d\xi_2}{dt} + x^0\frac{d\xi_1}{dt} = x_1\mu_1 + x_2\mu_2 - \frac{1}{2}x^0\frac{F^0}{V^0}\xi_1 - F^0\xi_2 \qquad\qquad 71$$

Subtract Eq.70 from 71,

$$V^0 \frac{d\xi_2}{dt} + x^0(\mu_1 + \mu_2) = x_1\mu_1 + x_2\mu_2 - F^0\xi_2 \qquad 72$$

we get the model

$$x(t) = x^0 + \xi_2(t) \qquad 69$$

$$F = F^0 + \frac{1}{2}\frac{F^0}{V^0}\xi_1(t) \qquad 73$$

$$\frac{1}{2}\frac{F^0}{V^0}\xi_1 = F - F^0$$
$$\xi_2 = x - x^0$$

$$\frac{d\xi_1}{dt} = -\frac{1}{2}\frac{F^0}{V^0}\xi_1 + \mu_1 + \mu_2 \quad (70)$$

$$\frac{d\xi_2}{dt} = -\frac{F^0}{V^0}\xi_2 + \frac{(x_1\mu_1 + x_2\mu_2) - (\mu_1 + \mu_2)x^0}{V^0}$$

$$= -\frac{F^0}{V^0}\xi_2 + \frac{(x_1 - x^0)\mu_1 + (x_2 - x^0)\mu_2}{V^0} \quad (72)$$

Let

$$\underline{x} = \begin{bmatrix} \xi_1 \\ \xi_2 \end{bmatrix}$$

$$\dot{x} = \begin{bmatrix} \dot{\xi}_1 \\ \dot{\xi}_2 \end{bmatrix}$$

therefore,

$$\underline{\underline{P}} = \begin{bmatrix} -\dfrac{F^0}{2V^0} & 0 \\ 0 & -\dfrac{F^0}{V^0} \end{bmatrix} \qquad \underline{\underline{B}} = \begin{bmatrix} 1 & 1 \\ \dfrac{x_1 - x^0}{V^0} & \dfrac{x_2 - x^0}{V^0} \end{bmatrix}$$

$$F_1(t) = F_1^0 + \mu_1(t) \qquad 66$$
$$F_2(t) = F_2^0 + \mu_2(t) \qquad 67$$

$$\underline{u} = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix} = \begin{bmatrix} F_1 - F_1^0 \\ F_2 - F_2^0 \end{bmatrix}$$

$$\frac{1}{2}\frac{F^0}{V^0}\xi_1 = F - F^0$$
$$\xi_2 = x - x^0$$

$$\underline{C} = \begin{bmatrix} F - F^0 \\ x - x^0 \end{bmatrix} \qquad \underline{\underline{L}} = \begin{bmatrix} \dfrac{F^0}{2V^0} & 0 \\ 0 & 1 \end{bmatrix}$$

Quiz VII

Consider the liquid-level system shown in the following Figure. In the system, $\overline{Q}_1$ and are $\overline{Q}_2$ steady-state inflow rates and $\overline{H}_1$ and $\overline{H}_2$ are steady state heads. The quantities q_{i1} q_{i2}, h_1, h_2, q_1 and q_o are considered small. Obtain a state-space representation of the system when h_1 and h_2 are the outputs and q_1 and q_2 are the inputs.
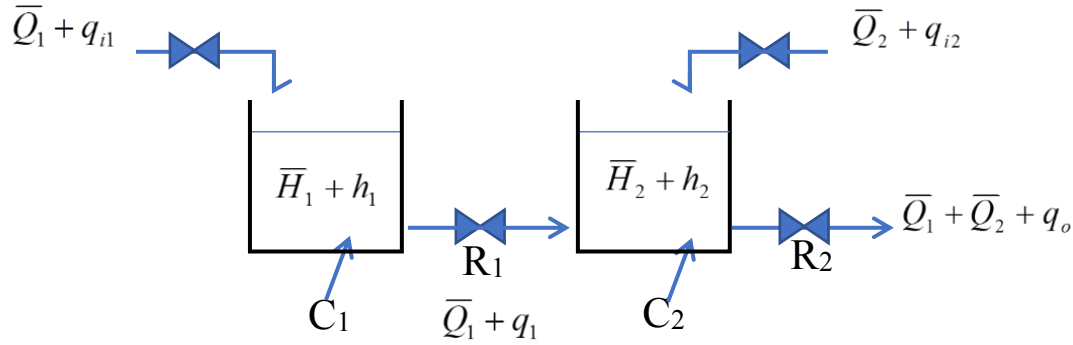
Solution: From the Figure,

$$C_1 \frac{d(\overline{H}_1 + h_1)}{dt} = (\overline{Q}_1 + q_{i1}) - (\overline{Q}_1 + q_1)$$

$$C_1 \frac{d(h_1)}{dt} = (q_{i1}) - (q_1)$$

$$C_2 \frac{d(h_2)}{dt} = (q_1) + (q_{i2}) - (q_o)$$

At the same time, for tank 1,

$$\frac{H_1 - H_2}{R_1} = Q_1, \text{ that is,}$$

$$\frac{(\overline{H}_1 + h_1) - (\overline{H}_2 + h_2)}{R_1} = \frac{(\overline{H}_1 - \overline{H}_2) + (h_1 - h_2)}{R_1} = \overline{Q}_1 + q_1, \text{ or}$$

$$\frac{(\overline{H}_1 - \overline{H}_2) + (h_1 - h_2)}{R_1} = \overline{Q}_1 + q_1, \text{ then } \frac{(\overline{H}_1 - \overline{H}_2)}{R_1} = \overline{Q}_1 \qquad \text{and } \frac{(h_1 - h_2)}{R_1} = q_1$$

Similarly for tank 2,

$$\frac{H_2}{R_2} = Q_2, \text{ that is } \frac{(\overline{H}_2 + h_2)}{R_2} = \overline{Q}_2 + q_o, \text{ therefore,}$$

$$\frac{(\overline{H}_2)}{R_2} = \overline{Q}_2 \qquad \text{and } \frac{(h_2)}{R_2} = q_o.$$

Therefore, we arrive at,

$$C_1 \frac{d(h_1)}{dt} = \left(q_{i1} - \frac{h_1 - h_2}{R_1} \right);$$

$$C_2 \frac{d(h_2)}{dt} = \left(q_{i2} + \frac{h_1 - h_2}{R_1} - \frac{h_2}{R_2} \right).$$

Define state variables as

$$\underline{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} h_1 \\ h_2 \end{bmatrix}$$

Input variables as

$$\underline{u} = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} q_{i1} \\ q_{i2} \end{bmatrix}$$

Output variable

$$\underline{c} = \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} h_1 \\ h_2 \end{bmatrix}$$

Then

$$\dot{x}_1 = -\frac{1}{R_1 C_1} x_1 + \frac{1}{R_1 C_1} x_2 + \frac{1}{C_1} u_1$$
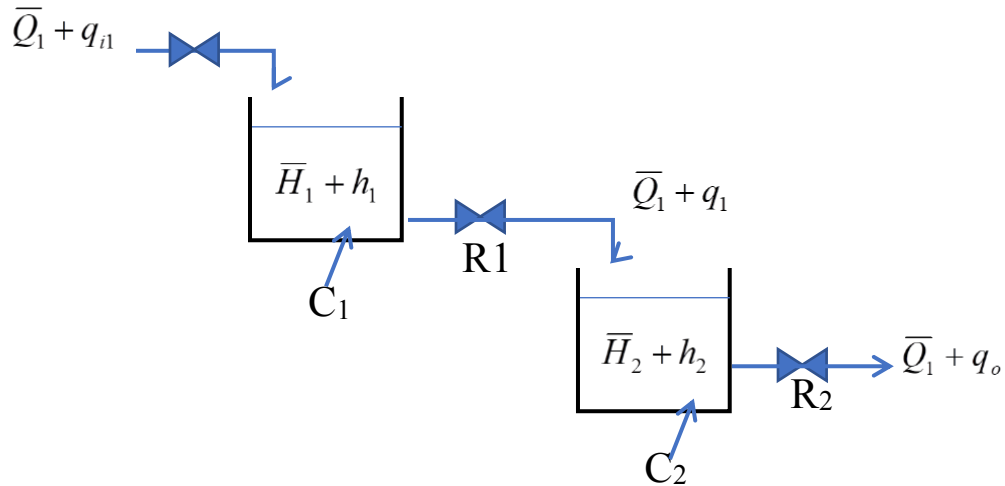
$$\dot{x}_2 = \frac{1}{R_1 C_2} x_1 - \left(\frac{1}{R_1 C_2} + \frac{1}{R_2 C_2} \right) x_2 + \frac{1}{C_2} u_2$$

$$\underline{\dot{x}} = \underline{\underline{P}} \underline{x} + \underline{\underline{B}} \underline{u}$$

$$\underline{\underline{P}} = \begin{bmatrix} -\dfrac{1}{R_1 C_1} & \dfrac{1}{R_1 C_1} \\ \dfrac{1}{R_1 C_2} & -\left(\dfrac{1}{R_1 C_2} + \dfrac{1}{R_2 C_2} \right) \end{bmatrix} \quad ; \quad \underline{\underline{B}} = \begin{bmatrix} \dfrac{1}{C_1} & 0 \\ 0 & \dfrac{1}{C_2} \end{bmatrix}$$

$$\underline{c} = \underline{\underline{L}} \underline{x}$$

$$\underline{\underline{L}} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Rate of accumulation = in -out

$$C_1 \frac{d(h_1)}{dt} = \left(q_{i1} - \frac{h_1}{R_1} \right);$$

$$C_2 \frac{d(h_2)}{dt} = \left(\frac{h_1}{R_1} - \frac{h_2}{R_2} \right).$$

Define state variables as

$$\underline{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} h_1 \\ h_2 \end{bmatrix}$$

Input variables as

$$\underline{u} = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} q_{i1} \\ 0 \end{bmatrix}$$

Output variable

$$\underline{c} = \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} h_1 \\ h_2 \end{bmatrix}$$

Then

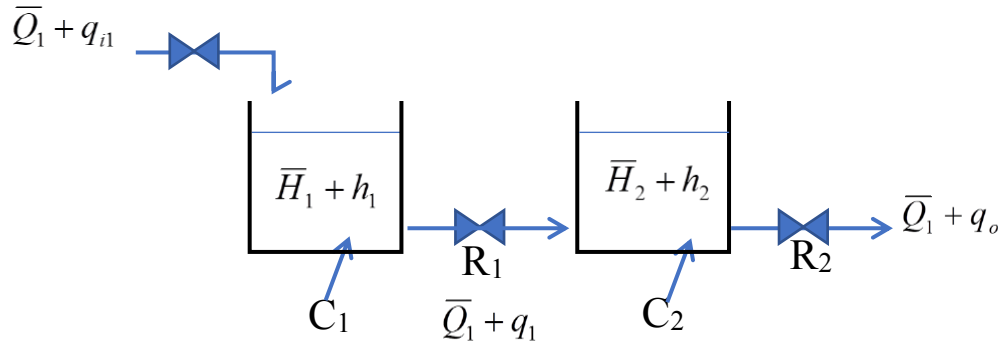$$\dot{x}_1 = -\frac{1}{R_1 C_1} x_1 + \frac{1}{C_1} u_1$$

$$\dot{x}_2 = \frac{1}{R_1 C_2} x_1 - \frac{1}{R_2 C_2} x_2$$

$$\underline{\dot{x}} = \underline{\underline{P}}\underline{x} + \underline{\underline{B}}\underline{u}$$

$$\underline{\underline{P}} = \begin{bmatrix} -\dfrac{1}{R_1 C_1} & 0 \\ \dfrac{1}{R_1 C_2} & -\dfrac{1}{R_2 C_2} \end{bmatrix} \quad ; \quad \underline{\underline{B}} = \begin{bmatrix} \dfrac{1}{C_1} & 0 \\ 0 & 0 \end{bmatrix}$$

$$\underline{c} = \underline{\underline{L}}\underline{x}$$

$$\underline{\underline{L}} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$C_1 \frac{d(h_1)}{dt} = \left(q_{i1} - \frac{h_1 - h_2}{R_1} \right);$$

$$C_2 \frac{d(h_2)}{dt} = \left(\frac{h_1 - h_2}{R_1} - \frac{h_2}{R_2} \right).$$

Define state variables as

$$\underline{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} h_1 \\ h_2 \end{bmatrix}$$

Input variables as

$$\underline{u} = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} q_{i1} \\ 0 \end{bmatrix}$$

Output variable

$$\underline{c} = \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} h_1 \\ h_2 \end{bmatrix}$$

Then

$$\dot{x}_1 = -\frac{1}{R_1 C_1} x_1 + \frac{1}{R_1 C_1} x_2 + \frac{1}{C_1} u_1$$

$$\dot{x}_2 = \frac{1}{R_1 C_2} x_1 - \left(\frac{1}{R_2 C_2} + \frac{1}{R_1 C_2} \right) x_2$$
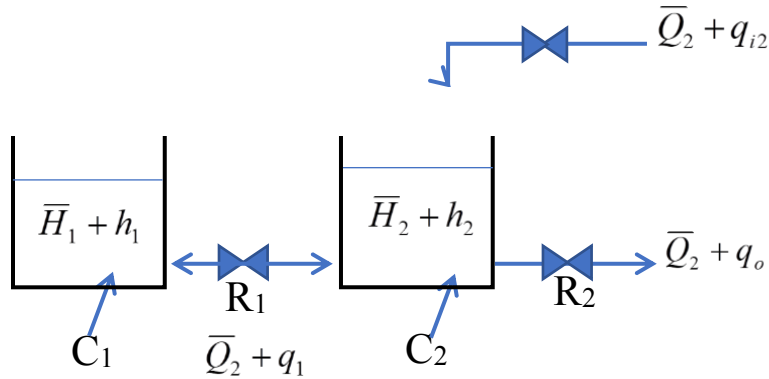
$$\underline{\dot{x}} = \underline{\underline{P}}\,\underline{x} + \underline{\underline{B}}\,\underline{u}$$

$$\underline{\underline{P}} = \begin{bmatrix} -\dfrac{1}{R_1 C_1} & \dfrac{1}{R_1 C_1} \\ \dfrac{1}{R_1 C_2} & -\left(\dfrac{1}{R_2 C_2} + \dfrac{1}{R_1 C_2} \right) \end{bmatrix} \quad ; \quad \underline{\underline{B}} = \begin{bmatrix} \dfrac{1}{C_1} & 0 \\ 0 & 0 \end{bmatrix}$$

$$\underline{c} = \underline{\underline{L}}\,\underline{x}$$

$$\underline{\underline{L}} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$C_1 \frac{d(h_1)}{dt} = -\left(\frac{h_1 - h_2}{R_1} \right);$$

$$C_2 \frac{d(h_2)}{dt} = \left(q_{i2} + \frac{h_1 - h_2}{R_1} - \frac{h_2}{R_2} \right).$$

Define state variables as

$$\underline{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} h_1 \\ h_2 \end{bmatrix}$$

Input variables as

$$\underline{u} = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} 0 \\ q_{i2} \end{bmatrix}$$

Output variable

$$\underline{c} = \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} h_1 \\ h_2 \end{bmatrix}$$

Then

$$\dot{x}_1 = -\frac{1}{R_1 C_1} x_1 + \frac{1}{R_1 C_1} x_2$$

$$\dot{x}_2 = \frac{1}{R_1 C_2} x_1 - \left(\frac{1}{R_2 C_2} + \frac{1}{R_1 C_2} \right) x_2 + \frac{1}{C_2} q_{i2}$$

$$\underline{\dot{x}} = \underline{\underline{P}}\,\underline{x} + \underline{\underline{B}}\,\underline{u}$$

$$\underline{\underline{P}} = \begin{bmatrix} -\dfrac{1}{R_1 C_1} & \dfrac{1}{R_1 C_1} \\ \dfrac{1}{R_1 C_2} & -\left(\dfrac{1}{R_2 C_2} + \dfrac{1}{R_1 C_2} \right) \end{bmatrix} \quad ; \qquad \underline{\underline{B}} = \begin{bmatrix} 0 & 0 \\ 0 & \dfrac{1}{C_2} \end{bmatrix}$$

$$\underline{c} = \underline{\underline{L}}\,\underline{x}$$

$$\underline{\underline{L}} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Answer

A $\quad \underline{\underline{P}} = \begin{bmatrix} -\dfrac{1}{R_1 C_1} & \dfrac{1}{R_1 C_1} \\ \dfrac{1}{R_1 C_2} & -\left(\dfrac{1}{R_1 C_2} + \dfrac{1}{R_2 C_2} \right) \end{bmatrix} ; \quad \underline{\underline{B}} = \begin{bmatrix} \dfrac{1}{C_1} & 0 \\ 0 & \dfrac{1}{C_2} \end{bmatrix}$

B $\quad \underline{\underline{P}} = \begin{bmatrix} -\dfrac{1}{R_1 C_1} & 0 \\ \dfrac{1}{R_1 C_2} & -\dfrac{1}{R_2 C_2} \end{bmatrix} ; \qquad \underline{\underline{B}} = \begin{bmatrix} \dfrac{1}{C_1} & 0 \\ 0 & 0 \end{bmatrix}$

C $\quad \underline{\underline{P}} = \begin{bmatrix} -\dfrac{1}{R_1 C_1} & \dfrac{1}{R_1 C_1} \\ \dfrac{1}{R_1 C_2} & -\left(\dfrac{1}{R_2 C_2} + \dfrac{1}{R_1 C_2} \right) \end{bmatrix} ; \quad \underline{\underline{B}} = \begin{bmatrix} \dfrac{1}{C_1} & 0 \\ 0 & 0 \end{bmatrix}$

D $\quad \underline{\underline{P}} = \begin{bmatrix} -\dfrac{1}{R_1 C_1} & \dfrac{1}{R_1 C_1} \\ \dfrac{1}{R_1 C_2} & -\left(\dfrac{1}{R_2 C_2} + \dfrac{1}{R_1 C_2} \right) \end{bmatrix} ; \quad \underline{\underline{B}} = \begin{bmatrix} 0 & 0 \\ 0 & \dfrac{1}{C_2} \end{bmatrix}$