Dynamic Process Modeling

Process Dynamics and Control

Process Modeling

- Description of process dynamics
  - Classes of models
  - What do we need for control?
- Modeling for control
  - Mechanical Systems Modeling
  - Electrical circuits and electrochemical systems
  - Fluid and heat flow models
- Brief intro to Matlab and Simulink tools (Tutorials 1 and 2)

Process Modeling

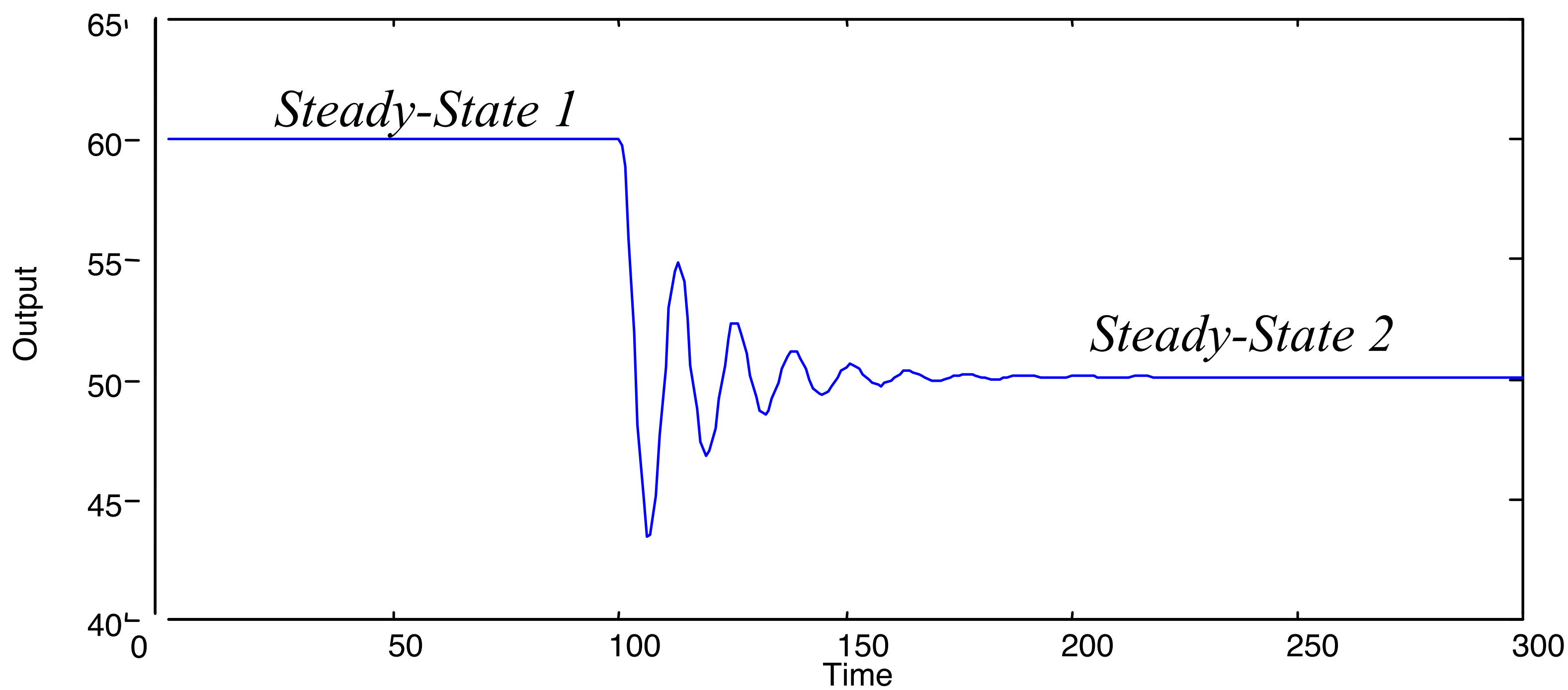
- Motivation:
  - Develop understanding of process
    - ➡ a mathematical hypothesis of process mechanisms
  - Match observed process behavior
    - ➡ useful in design, optimization and *control* of processes
- Control:
  - Interested in description of process dynamics
    - ➡ Dynamic model is used to predict how process responds to given input
    - ➡ Tells us how to react

What kind of model do we need?

- *Dynamic vs. Steady-state (Static)*
  - Steady-state (Static)
    - Variables not a function of time
    - useful for design calculation
  - *Dynamic*
    - Variables are a function of time
    - Control requires dynamic model

Process Modeling

- *Dynamic vs. Steady-state*



- *Step change in input to observe*
  - Starting at steady-state, we made a step change
  - The system oscillates and finds a new steady-state
  - ***Dynamics describe the transient behavior***

What kind of model do we need?

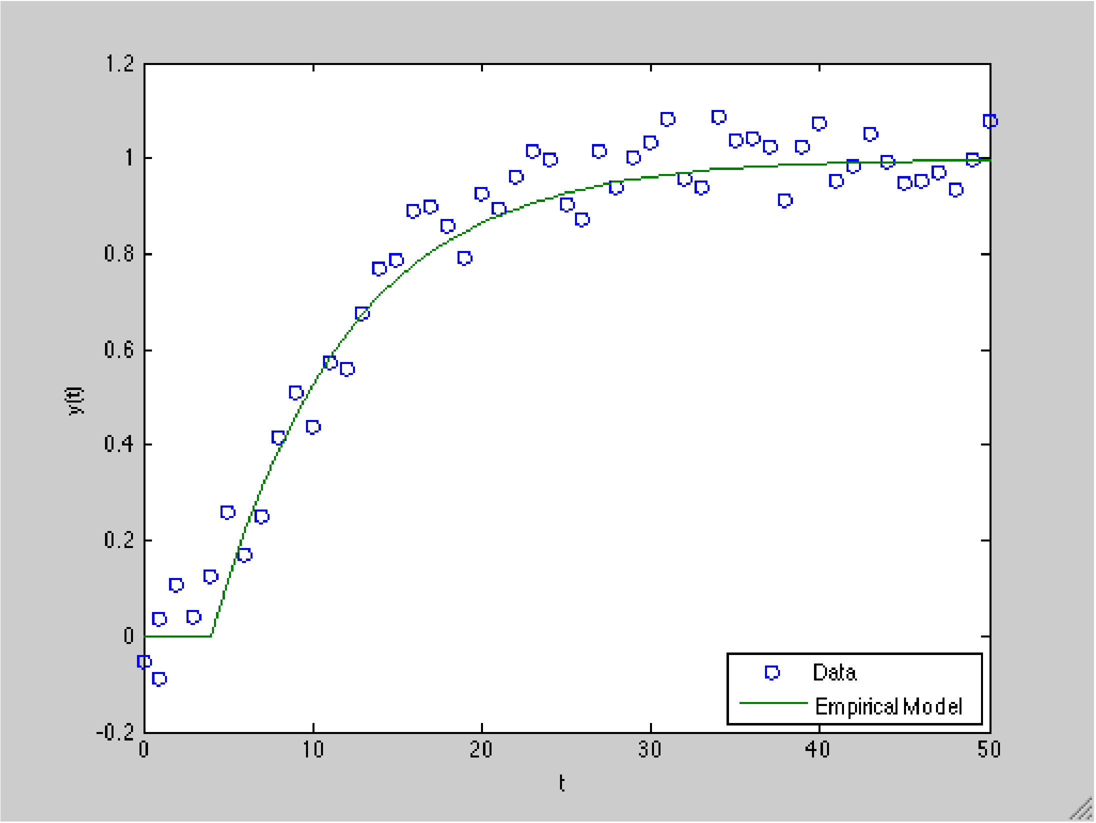
- *Experimental vs Theoretical*
  - Experimental
    - Derived from tests performed on actual process
    - Simpler model forms
    - Easier to manipulate
  - Theoretical
    - Application of fundamental laws
    - more complex but provides understanding
    - Required in design stages

Process Modeling

- Empirical vs. Mechanistic models
  - Empirical Models
    - only local representation of the process (no extrapolation)
    - model only as good as the data
  - Mechanistic Models
    - Rely on our understanding of a process
    - Derived from first principles
    - Observing physical laws
    - Useful for simulation and exploration of new operating conditions
    - May contain unknown constants that must be estimated

Process Modeling

- *Empirical vs Mechanistic models*
  - Empirical models
    - do not rely on underlying mechanisms
    - Fit specific function to match process



Process Modeling

- Mechanistic modeling procedure
  - Identify modeling objectives
    - end use of model (e.g. control)
  - Apply fundamental physical and chemical laws
    - Mass, Energy and/or Momentum balances
  - Make appropriate assumptions (Simplify)
    - ideality (e.g. isothermal, adiabatic, ideal gas, no friction, incompressible flow, etc,…)
  - Develop the model equations

- Modeling procedure
  - Check model consistency
    - do we have more unknowns than equations
  - Determine unknown constants
    - e.g. friction coefficients, fluid density and viscosity
  - Solve model equations
    - typically nonlinear ordinary (or partial) differential equations
    - initial value problems
  - Check the validity of the model
    - compare to process behavior

Process Modeling

- For control applications:
  - Modeling objectives is to describe process dynamics based on the laws of conservation of mass, energy and momentum
- The balance equation

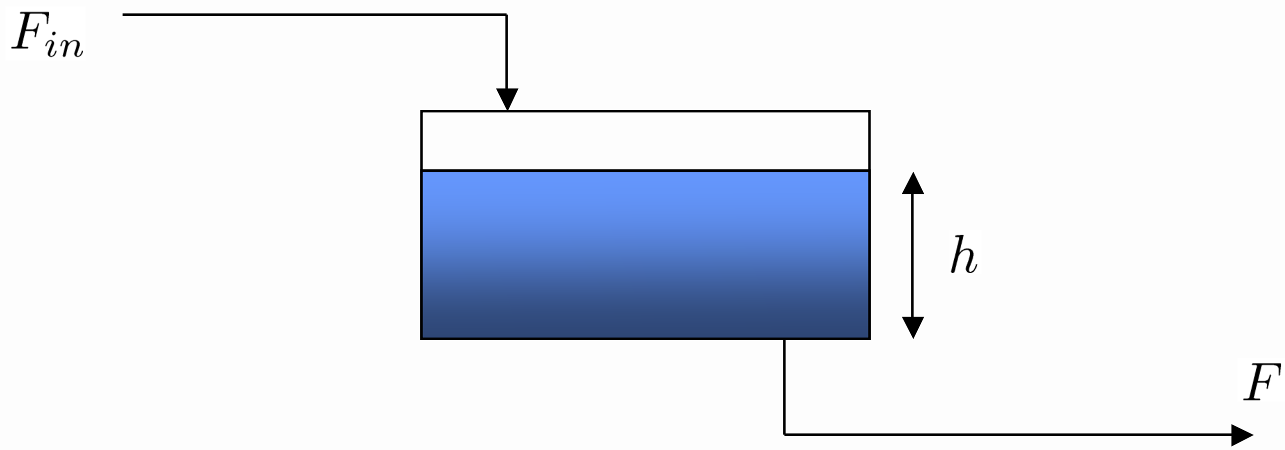
$$\begin{pmatrix} \textit{Rate of Accumulation} \\ \textit{of fundamental quantity} \end{pmatrix} = \begin{pmatrix} \textit{Flow} \\ \textit{In} \end{pmatrix} - \begin{pmatrix} \textit{Flow} \\ \textit{Out} \end{pmatrix} + \begin{pmatrix} \textit{Rate of} \\ \textit{Production} \end{pmatrix}$$

1. Mass Balance
2. Energy Balance
3. *Momentum Balance (Newton's Law)*

Process Modeling

- Application of a mass balance

  Holding Tank



- *Modeling objective*: Control of tank level
- *Fundamental quantity:* Mass
- *Assumptions*: Incompressible flow

Process Modeling

Total mass in system $= \rho V = \rho A h$

Flow in $= \rho F_{in}$

Flow out $= \rho F$

- Balance equation:

$$\frac{d\rho A h}{dt} = \rho F_{in} - \rho F$$

  - For constant density

$$\rho A \frac{dh}{dt} = \rho F_{in} - \rho F$$

$$\downarrow \left(\times \frac{1}{\rho A} \right)$$

$$\frac{dh}{dt} = \frac{1}{A} \left(F_{in} - F \right)$$

- Taking Laplace transform

$$sH(s) = \frac{1}{A}F_{in}(s) - \frac{1}{A}F(s)$$

$$\Big\downarrow \left(\times \frac{1}{s}\right)$$

$$H(s) = \frac{1}{As}F_{in}(s) - \frac{1}{As}F(s)$$

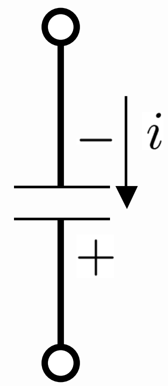
- If the outlet flow is zero ($F = 0$)

$$H(s) = \frac{1}{As}F_{in}(s)$$

- Interesting parallel with capacitor
  - Holding tank (assume $F = 0$)

$$\frac{H(s)}{F_{in}(s)} = \frac{1}{As}$$

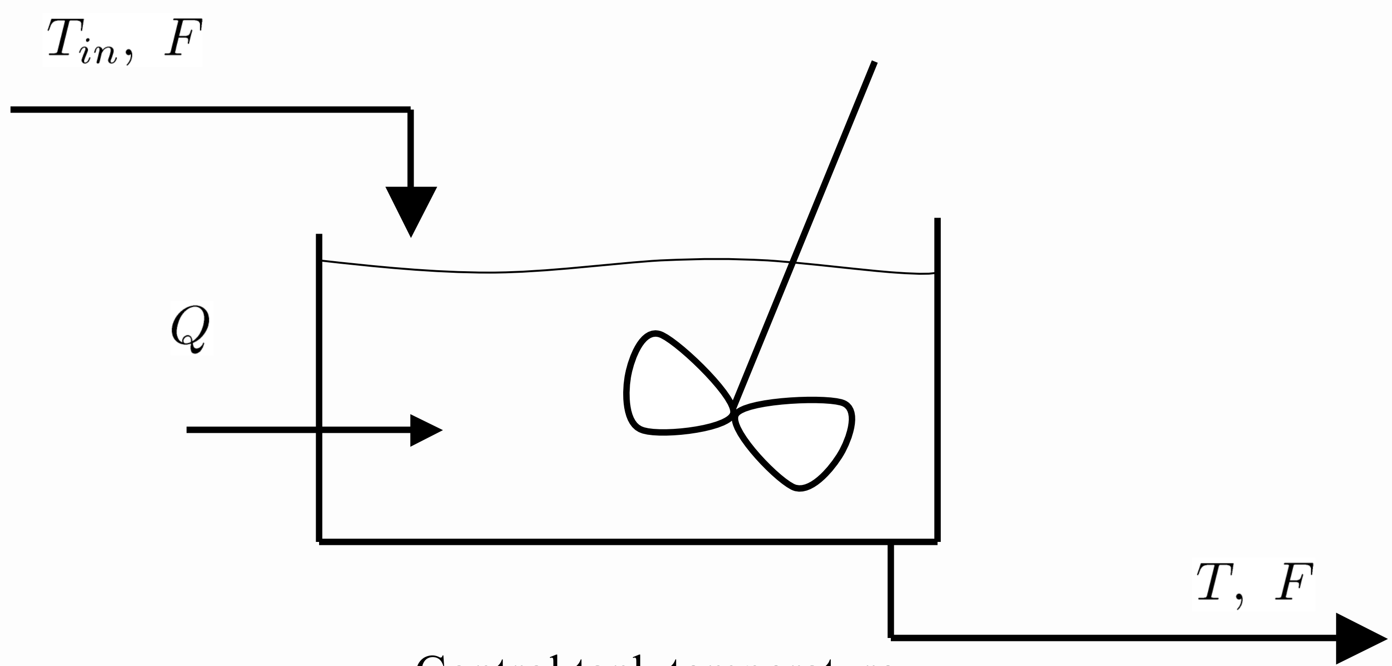
  - Capacitor



$$i = C\frac{dv}{dt} \rightarrow \frac{V(s)}{I(s)} = \frac{1}{Cs}$$

  - Dynamics of both systems are equivalent

- *Energy balance*



Objective:	Control tank temperature
Fundamental quantity:	Mass and Energy
Assumptions:	Incompressible flow
	Constant hold-up
	Constant mean pressure

Process Modeling

- Under constant hold-up and constant density
  - Mass balance equation
    - Total Mass ρV
    - Mass In ρF
    - Mass Out ρF

$$\frac{d\rho V}{dt} = \rho F - \rho F = 0$$

$$\frac{dV}{dt} = 0$$

  - Constant volume

Process Modeling

- Under constant hold-up and constant mean pressure changes
  - Energy Balance leads to an enthalpy balance

$$\frac{dH}{dt} = \dot{H}_{in} - \dot{H}_{out} + Q + W_s$$

  - Inlet Enthalpy $\dot{H}_{in} = \rho F C_p (T_{in} - T_{ref})$
  - Outlet Enthalpy $\dot{H}_{out} = \rho F C_p (T - T_{ref})$
  - Heat flow to the system Q
  - Work done on system $W_s (= 0)$
  - Total enthalpy in the system $H = \rho V C_p (T - T_{ref})$

$$\frac{d\rho V C_p (T - T_{ref})}{dt} = \rho F C_p (T_{in} - T_{ref}) - \rho F C_p (T - T_{ref}) + Q$$

After substitution,with T_{ref} fixed and assuming constant $\rho,\ C_p$

$$\rho C_p V \frac{dT}{dt} = \rho C_p F(T_{in} - T) + Q$$

Divide by $\rho C_p V$

$$\frac{dT}{dt} = \frac{F}{V}(T_{in} - T) + \frac{Q}{\rho C_p V}$$

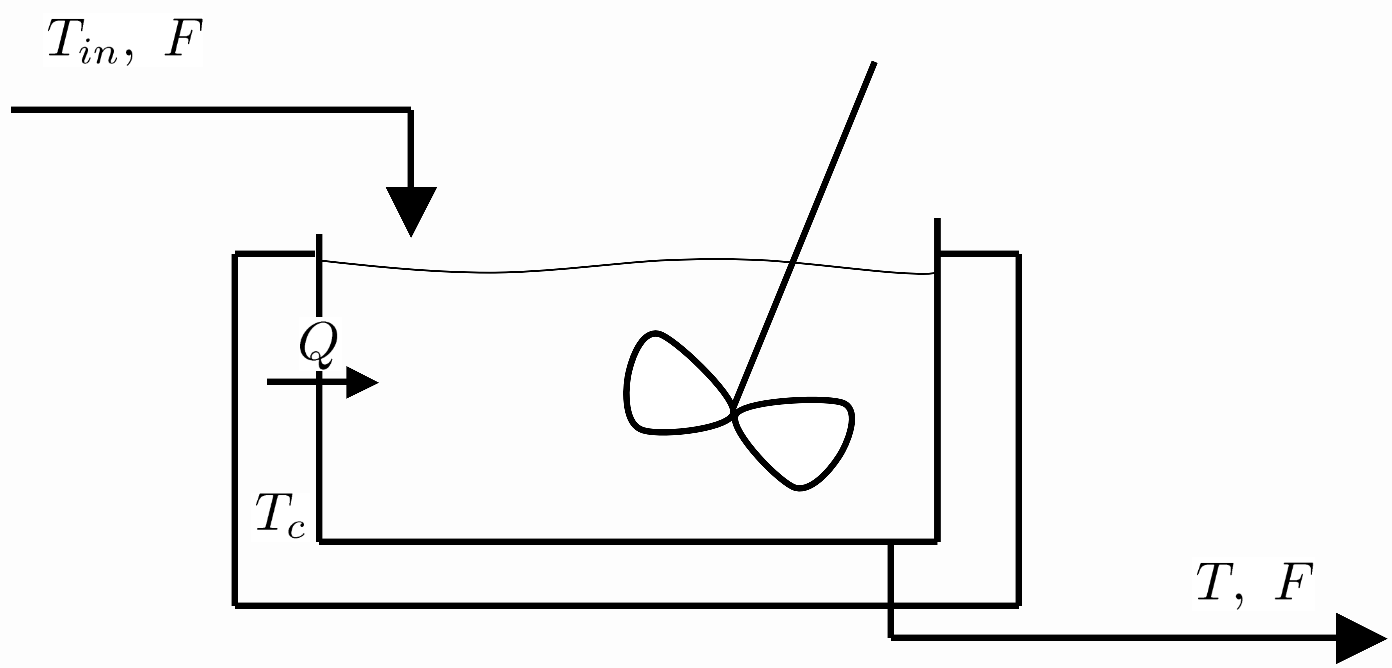
- *Heat input from a hot (or cold source) at temperature* T_c

$$Q = UA(T_c - T)$$

where U *is a heat-transfer coefficient*

A *is the effective area for heat transfer*

- Modeling heat input



- Heat input is proportional to the difference in temperature

$$Q = UA(T_c - T)$$

Assume F is fixed then the ODE is linear, use Laplace Transforms

$$sT(s) - T(0) = \frac{F}{V}T(s) + \frac{1}{\rho C_p V}Q(s)$$

where $\tau = V/F$ is the tank residence time (or time constant)

Isolating and solving for $T(s)$ gives

$$T(s) = \frac{1}{\tau s+1}T(0) + \frac{\frac{1}{\rho C_p V}}{\tau s+1}Q(s)$$

If F changes with time then the differential equation does not have a closed form solution.

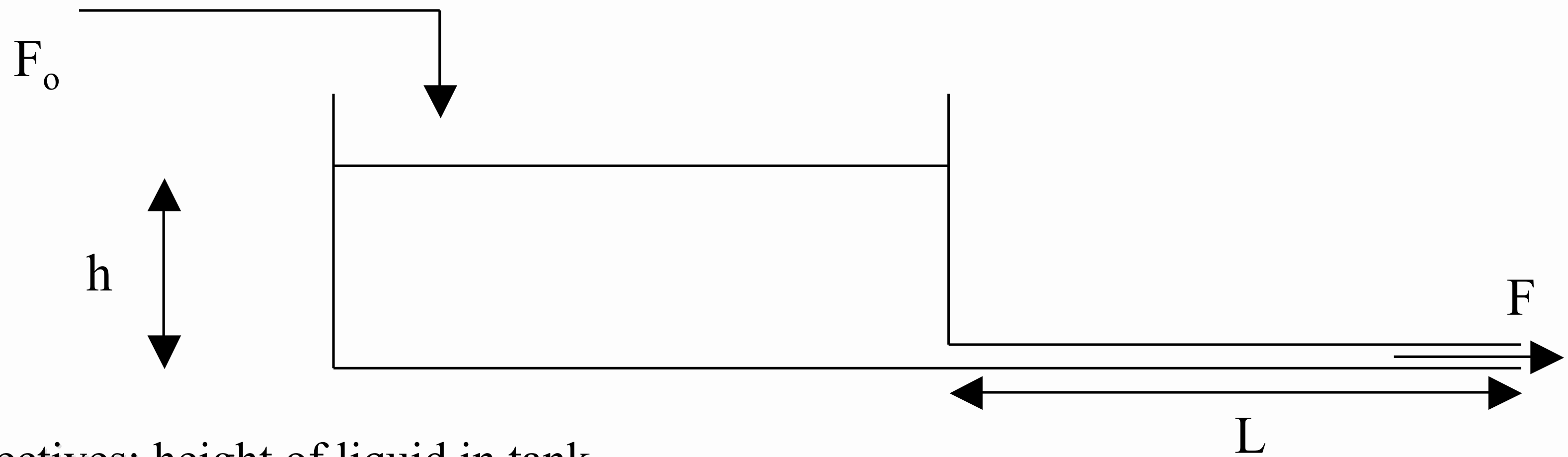
$$\frac{dT}{dt} = \frac{F(t)}{V}(T_{in}(t) - T(t)) + \frac{Q(t)}{\rho C_p V}$$

Products $F(t)T_{in}(t)$ and $F(t)T(t)$ makes this differential equation *nonlinear*.

Solution will need *numerical integration*.

Process Modeling

- Gravity tank



Objectives: height of liquid in tank

Fundamental quantity: Mass, momentum

Assumptions:

- Outlet flow is driven by head of liquid in the tank
- Incompressible flow
- Plug flow in outlet pipe
- Turbulent flow

Process Modeling

From mass balance and Newton's law,

$$\frac{dh}{dt} = \frac{F_o}{A} - \frac{A_p v}{A}$$
$$\frac{dv}{dt} = \frac{hg}{L} - \frac{K_f v^2}{\rho A_p L}$$

A *system* of *simultaneous* ordinary differential equations results

Linear or nonlinear?

Solution of ODEs

- Mechanistic modeling results in (sets of) nonlinear ordinary differential equations

- Solution requires numerical integration

- To get solution, we must first:
  - specify all constants
  - specify all initial conditions
  - specify types of perturbations of the input variables

For the heated stirred tank,

$$\frac{dT}{dt} = \frac{F}{V}(T_{in} - T) + \frac{Q}{\rho C_p V}$$

- specify $\rho,\ C_p,\ V$
- specify $T(0)$
- specify $Q(t),\ F(t)$

Input Specifications

- Study of control system dynamics
  - Observe the time response of a process output in response to input changes

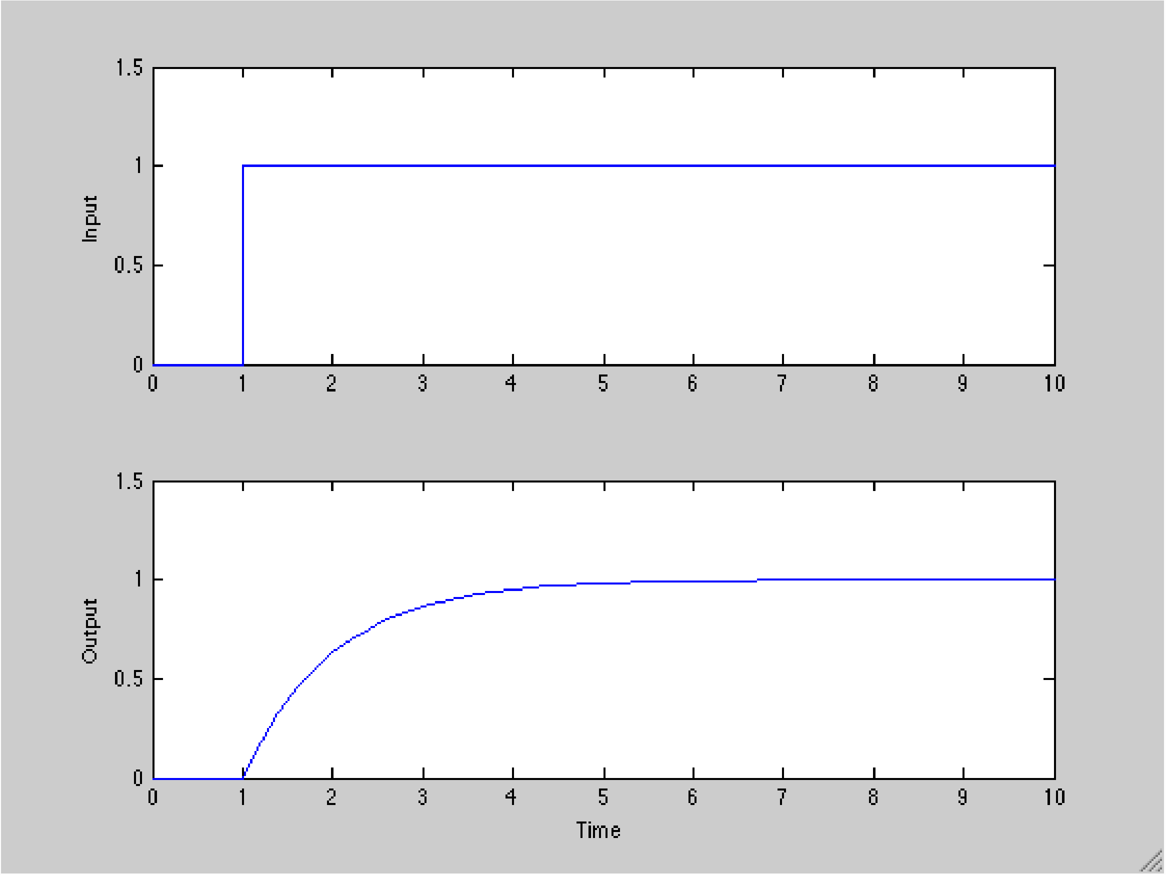
- Focus on specific inputs

1. Step input signals
2. Ramp input signals
3. Pulse and impulse signals
4. Sinusoidal signals
5. Random (noisy) signals

Common Input Signals

1. Step Input Signal: a sustained instantaneous change

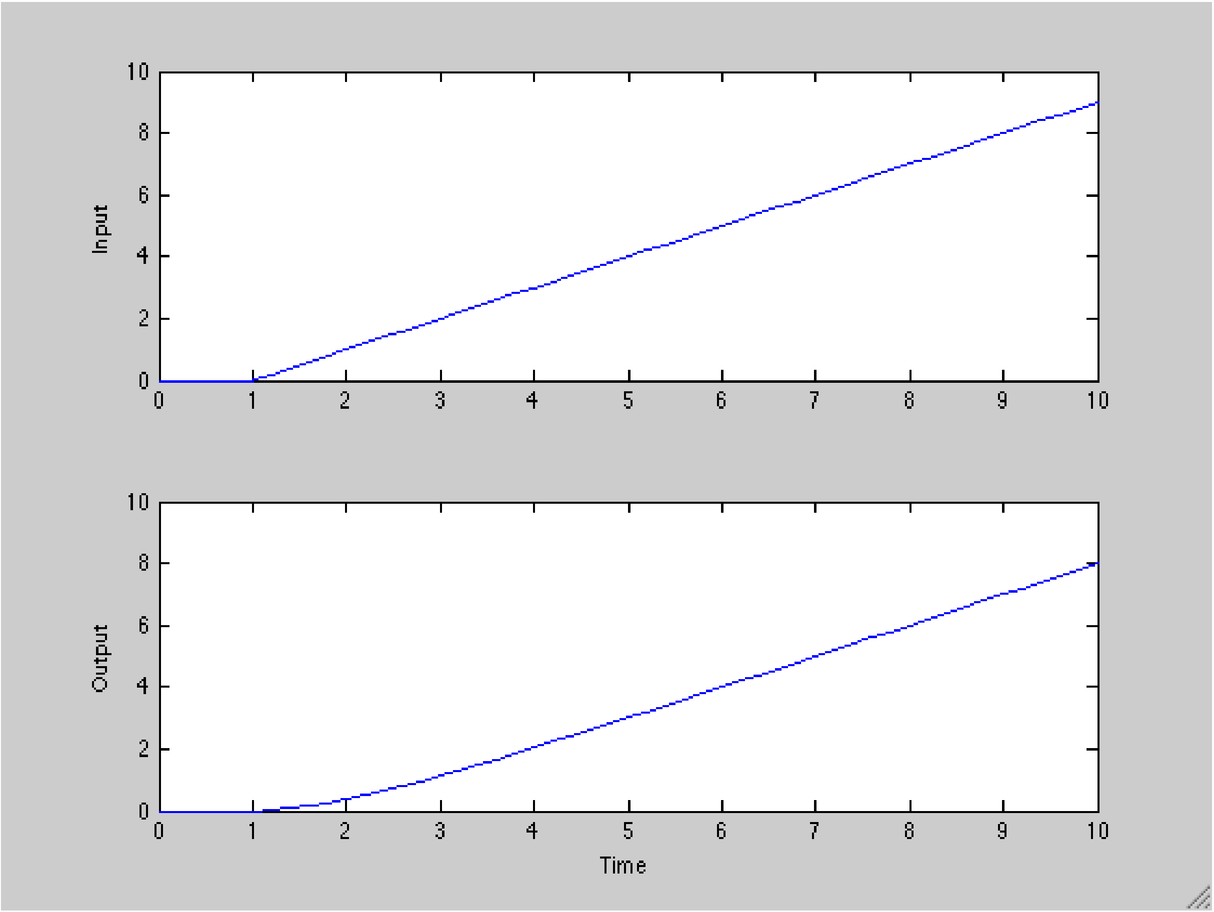
e.g. Unit step input introduced at time 1



Common Input Signals

2. Ramp Input: A sustained constant rate of change

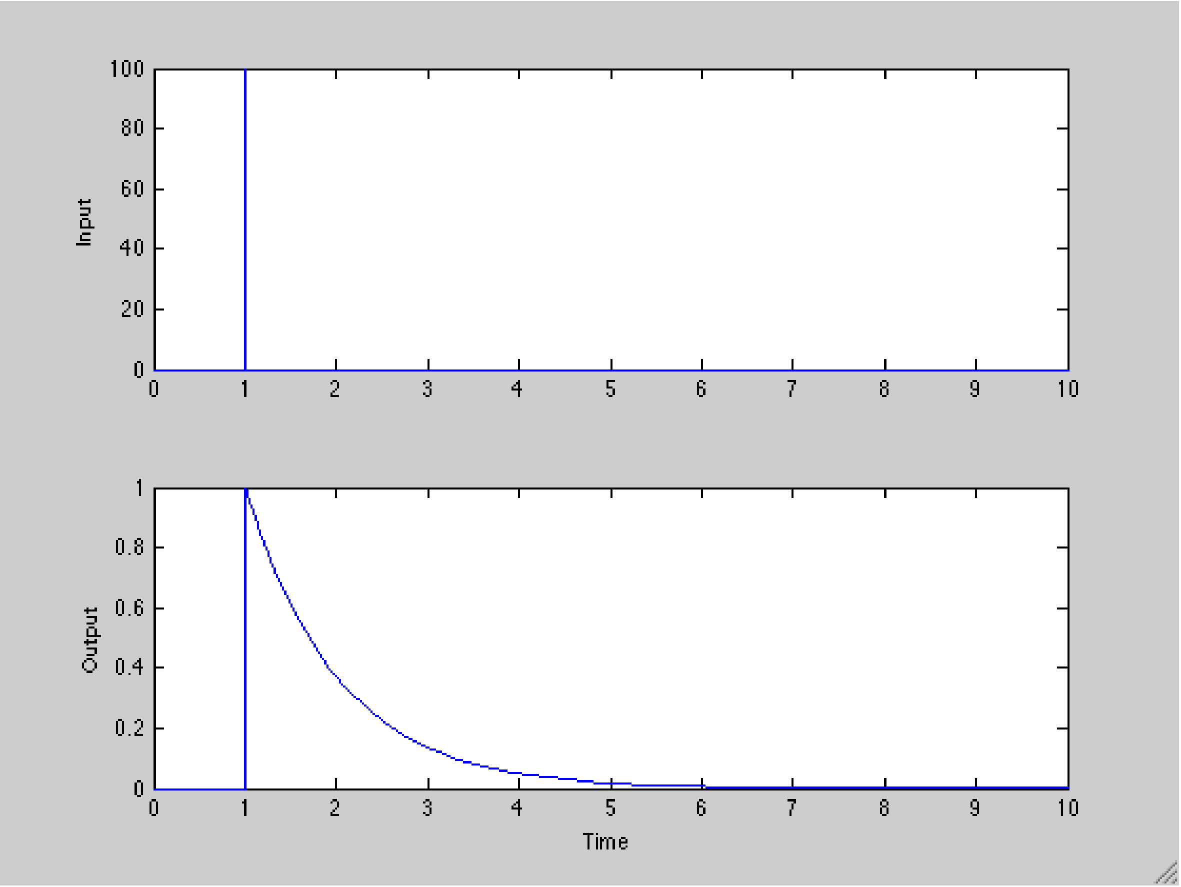
e.g. Ramp input at time t=1



Common Input Signals

3. Pulse: An instantaneous temporary change

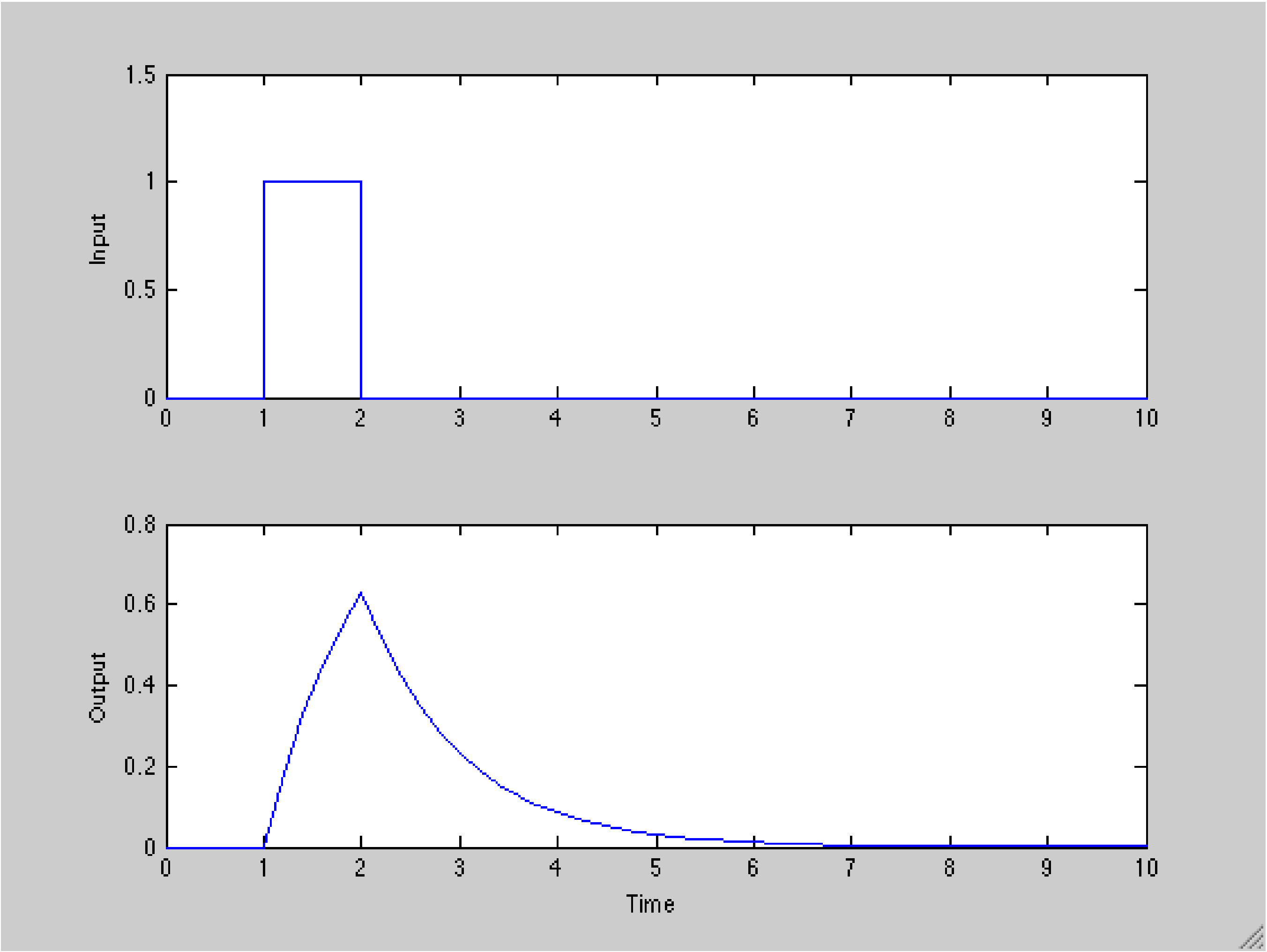
e.g. Fast pulse (unit impulse) at t=1



Common Input Signals

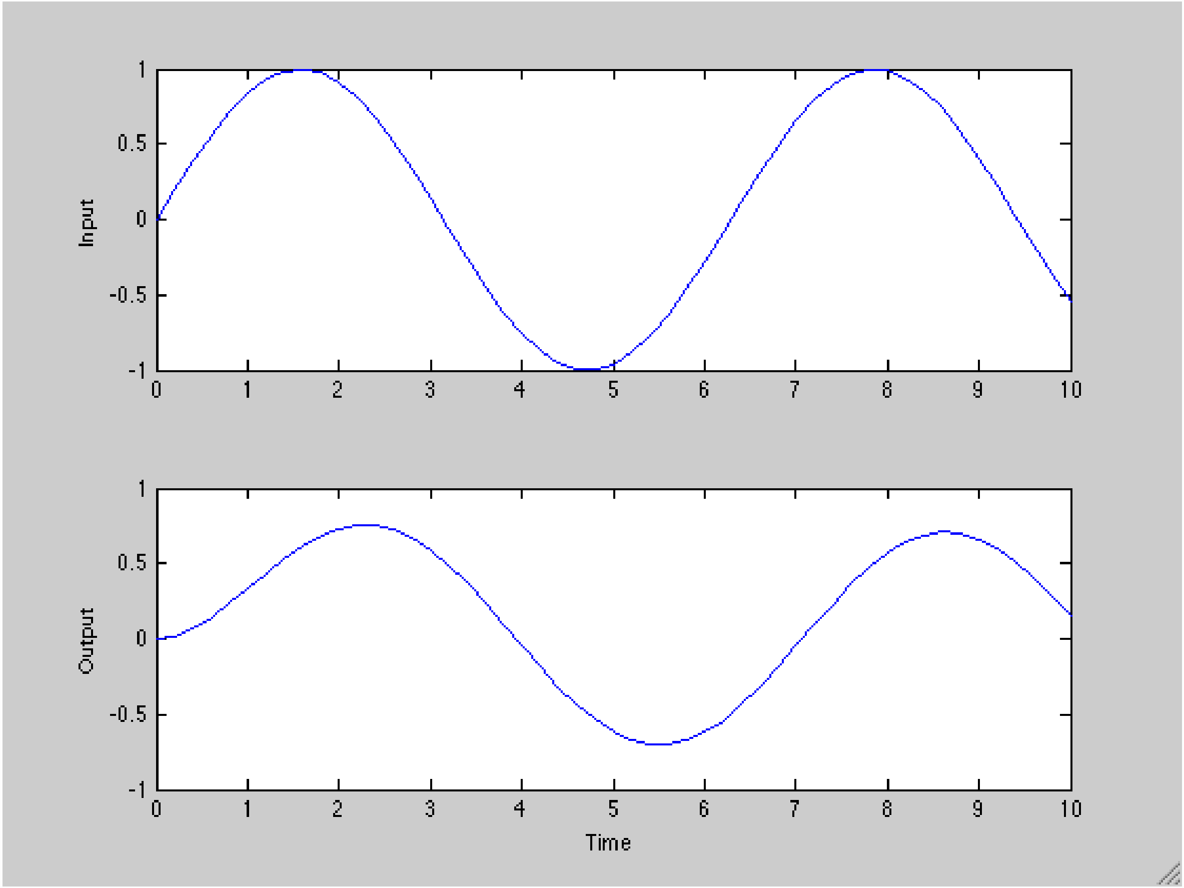
3. Pulses:

e.g. Rectangular Pulse



Common Input Signals

4. Sinusoidal input, e.g. $u(t) = \sin t$



Common Input Signals

5. Random Input, e.g. white noise