

# Master in Control Engineering

## Process Automation 2020-2021

DIPARTIMENTO DI INGEGNERIA INFORMATICA  
AUTOMATICA E GESTIONALE ANTONIO RUBERTI



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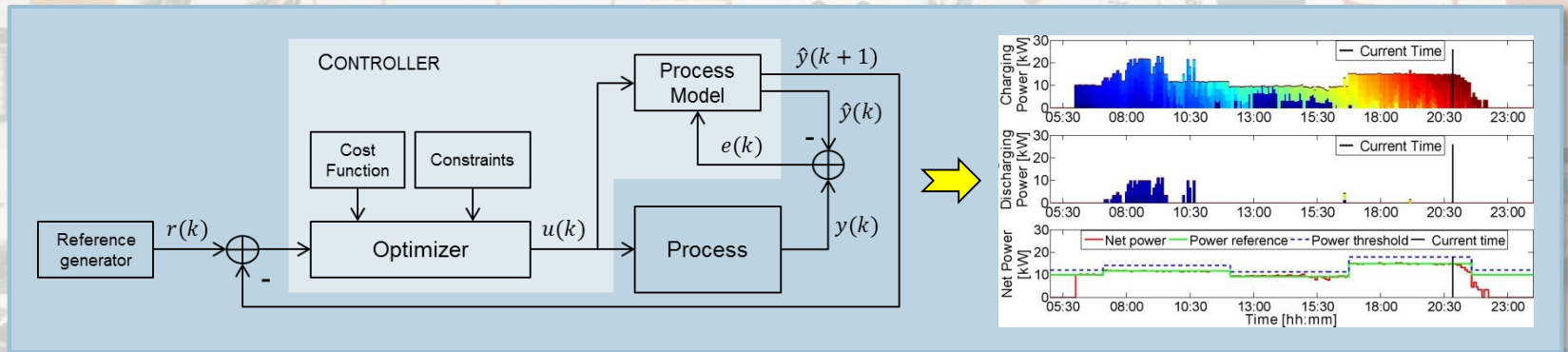
# Master in Control Engineering

## Process Automation

### 4. DYNAMIC PROCESS MODELS

Slides based on:

D.E. Seborg et al., *Process Dynamics and Control* (3<sup>rd</sup> ed.), 2009, Ch. 2



# Outline

- Dynamic Process Models
  - Why use dynamic models?
  - Classification
  - Modelling principles
  - Conservation laws
    - Degrees of freedom
  - Examples of process control models
    - Blending process control
    - Stirred-tank heating process
    - Liquid storage system
    - Fed-batch (semi-continuous) bioreactor
  - Linearization of nonlinear models
    - Blending process control
- Summary

# Why use dynamic models?

- 1. *Improve understanding of the process*
  - Dynamic models and computer simulations allow transient process behavior to be investigated without operating the process
  - Computer simulations are used to acquire valuable information about dynamic and steady-state process behavior, even before the plant is constructed
- 2. *Train plant operating personnel*
  - Process simulators play a critical role in training plant operators to run complex units and to deal with emergency situations
  - A realistic training environment is created by interfacing a process simulator to standard process control equipment

# Why use dynamic models?

- 3. *Develop a control strategy for a new process*
  - Alternative control strategies can be evaluated over a dynamic model of the process
    - Help to identify the process variables that should be controlled and those that should be manipulated
    - Allows model-based control strategies to be employed, in which the process model is part of the control law.
- 4. *Optimize process operating conditions*
  - A steady-state process model and economic information can be used to determine the most profitable operating conditions
  - It also allows recalculating the optimum operating conditions periodically in order to maximize profit

# Classification

- Models can be classified based on how they are obtained
  - (a) Theoretical models
    - Developed using the principles of chemistry, physics, and biology
    - Advantages
      - Physical insight into process behavior
      - Applicable over wide ranges of conditions
    - Disadvantages
      - Expensive and/or time-consuming to develop
      - Theoretical models of complex processes typically include some model parameters that are not readily available
        - » reaction rate coefficients, physical properties, heat transfer coefficients

# Classification

- Models can be classified based on how they are obtained
  - (b) Empirical models
    - Obtained by fitting experimental data
    - Advantage
      - Easier to develop than theoretical models
    - Disadvantage
      - Do not extrapolate well
        - » Empirical models should be used with caution for operating conditions that were not included in the experimental data used to fit the model
        - » The range of the data is typically quite small compared to the full range of process operating conditions.
  - (c) Semi-empirical models
    - Combination of the models in categories (a) and (b)
    - The numerical values of one or more of the parameters in a theoretical model are calculated from experimental data
    - May overcome the disadvantages of the other categories

# Modelling Principles

- A process model is a mathematical abstraction of a real process
  - The model equations are at best an approximation to the real process
    - It cannot incorporate all of the features of the real process
      - Compromise between
        - » accuracy and complexity
        - » cost and effort required to develop the model and to verify it
    - The model should incorporate all of the important dynamic behavior while being no more complex than is necessary
      - Omission of less important phenomena to keep the number of model equations, variables, and parameters low
  - Dynamic models of chemical processes consist of ordinary differential equations (ODE) and/or partial differential equations (PDE), plus related algebraic equations
    - For process control problems, dynamic models are derived using unsteady-state conservation laws
    - System of Differential-Algebraic Equations (DAE)
      - Algebraic equations = constraints over state variables



# Modelling principles

- Systematic approach for developing dynamic models
  1. State the modeling objectives and determine the required levels of model detail and accuracy
  2. Draw a schematic diagram of the process and label all process variables
  3. List all of the assumptions involved in developing the model
  4. Determine whether spatial variations of process variables are important (which requires a partial differential equation model)
  5. Write conservation equations (mass, component, energy, ...)
  6. Introduce equilibrium relations and other algebraic equations (from thermodynamics, transport phenomena, chemical kinetics, ..)
  7. Perform a degrees of freedom analysis to ensure that the model equations can be solved
  8. Simplify the model by rearranging the equations so that the output variables appear on the left side and the input variables appear on the right side
  9. Classify inputs as disturbance variables or as manipulated variables.

# Conservation Laws

- *Conservation of mass*

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

- *Conservation of component*

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

- Rate of comp.  $i$  produced represents the rate of generation (or consumption) of component  $i$  as a result of chemical reactions
- Conservation equations are also written in terms of molar quantities, atomic species, and molecular species

# Conservation Laws

- *Conservation of energy*
  - First law of thermodynamics

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

- The total energy of a thermodynamic system  $U_{tot}$  is the sum of its internal energy, kinetic energy, and potential energy

$$U_{tot} = U_{int} + U_{KE} + U_{PE}$$

# Conservation Laws

- *Conservation of energy*
  - First law of thermodynamics

$$\left\{ \begin{array}{l} \text{rate of energy} \\ \text{accumulation} \end{array} \right\} = \left\{ \begin{array}{l} \text{rate of energy in} \\ \text{by convection} \end{array} \right\} - \left\{ \begin{array}{l} \text{rate of energy out} \\ \text{by convection} \end{array} \right\}$$

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

- The total energy of a thermodynamic system  $U_{tot}$  is the sum of its internal energy, kinetic energy, and potential energy

$$U_{tot} = U_{int} + U_{KE} + U_{PE}$$

- Assumptions
  - Changes in potential energy and kinetic energy are small in comparison with changes in internal energy and can be neglected
  - The net rate of work is small compared to the rates of heat transfer and convection and can be neglected

# Conservation Laws

- *Conservation of energy*
  - First law of thermodynamics

$$\left\{ \begin{array}{l} \text{rate of energy} \\ \text{accumulation} \end{array} \right\} = \underbrace{\left\{ \begin{array}{l} \text{rate of energy in} \\ \text{by convection} \end{array} \right\} - \left\{ \begin{array}{l} \text{rate of energy out} \\ \text{by convection} \end{array} \right\}}_{-\Delta(w\hat{H})} + \left\{ \begin{array}{l} \text{net rate of heat addition} \\ \text{to the system from} \\ \text{the surroundings} \end{array} \right\}$$
$$\frac{dU_{int}}{dt} = -\Delta(w\hat{H}) + Q$$

$U_{int}$ : internal energy of the thermodynamic system

$w$ : mass flow rate (0 for batch processes)

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

$Q$ : rate of heat transfer to the system

- Expressions for  $U_{int}$ ,  $\hat{H}$  and  $Q$  are derived from thermodynamics

# Degrees of freedom

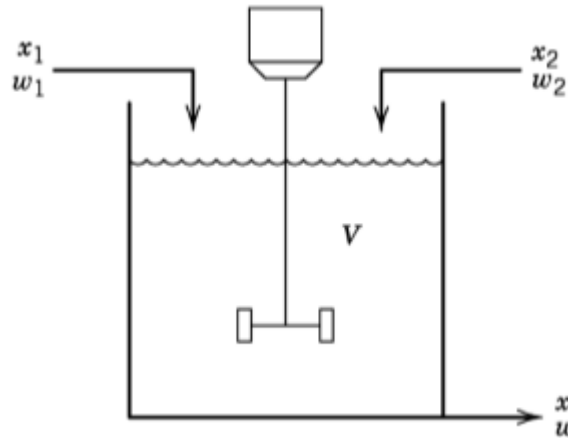
- The model equations should constitute a solvable set of relations
  - The output variables can be solved in terms of the input variables
- In order for the model to have a unique solution, the number of unknown variables must equal the number of independent model equations
  - All of the available degrees of freedom must be utilized
- Number of degrees of freedom  $N_F$ 
$$N_F = N_V - N_E$$

$N_V$ : total number of process variables  
 $N_E$ : number of independent equations
- 1.  $N_F = 0$ : the process model is exactly specified.
  - The set of equations has a solution (not necessarily unique for nonlinear equations)
- 2.  $N_F > 0$ : the process is underspecified
  - More process variables than equations (infinite number of solutions)
- 3.  $N_F < 0$ : The process model is overspecified
  - Fewer process variables than equations (no solution)

# Degrees of Freedom

- Degrees of Freedom Analysis
  1. List all quantities in the model that are known constants (or parameters that can be specified) on the basis of equipment dimensions, known physical properties, ...
  2. Determine the number of equations  $N_E$  and the number of process variables  $N_V$
  3. Calculate the number of degrees of freedom  $N_F = N_V - N_E$
  4. Identify the  $N_E$  output variables that will be obtained by solving the process model
  5. Identify the  $N_F$  input variables that must be specified as either disturbance variables or manipulated variables, in order to utilize the  $N_F$  degrees of freedom

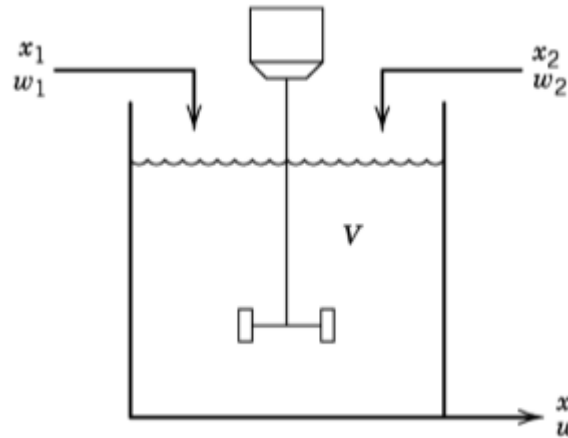
## Example: blending process control



- Control objective
  - Blend the two inlet streams to produce an outlet stream with desired composition
- Streams 1 and 2
  - A mixture of two chemical species, A and B, with total mass flow rates  $w_1(t)$  and  $w_2(t)$
  - Mass fractions of A  $x_1(t)$  and  $x_2(t)$  vary with time
- Volume of liquid in the tank  $V(t)$  varies with time

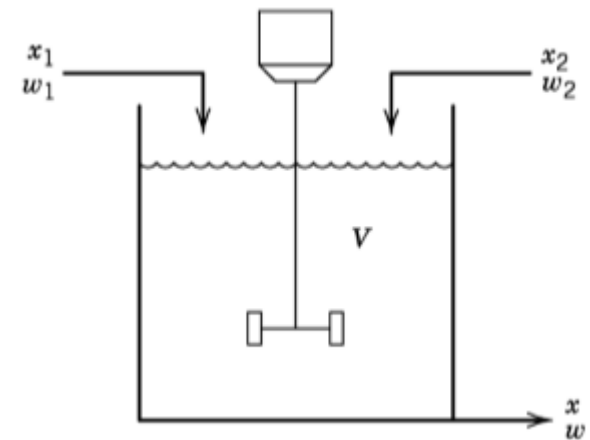


## Example: blending process control



- Assumptions
  - Perfect mixing assumption
    - (i) there are no concentration gradients in the tank
    - (ii) the composition of the exit stream is equal to the tank composition
      - » Assumption valid for low-viscosity liquids that receive an adequate degree of agitation
  - The density of the liquid  $\rho$  is constant
- Compute the static and dynamic models

## Example: blending process control



- Unsteady mass balance

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

- Rate of mass accumulation in the tank

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

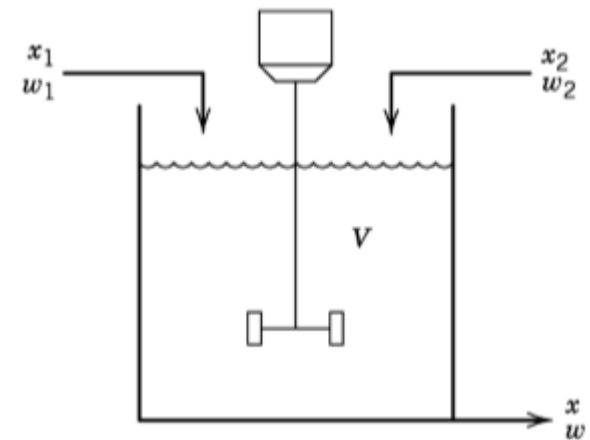
- Perfect mixing assumption

- Rate of mass accumulation for component A is proportional to the total rate of accumulation

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

- (1)-(2): unsteady-state model for the blending system

## Example: blending process control



- Static model

- The steady-state model is obtained by setting the accumulation terms to 0 (barred variables stands for the nominal value) in eq. (1) and (2):

$$\bar{w}_1 + \bar{w}_2 - \bar{w} = 0 \quad (1')$$

$$\bar{w}_1 \bar{x}_1 + \bar{w}_2 \bar{x}_2 - \bar{w} \bar{x} = 0 \quad (2')$$

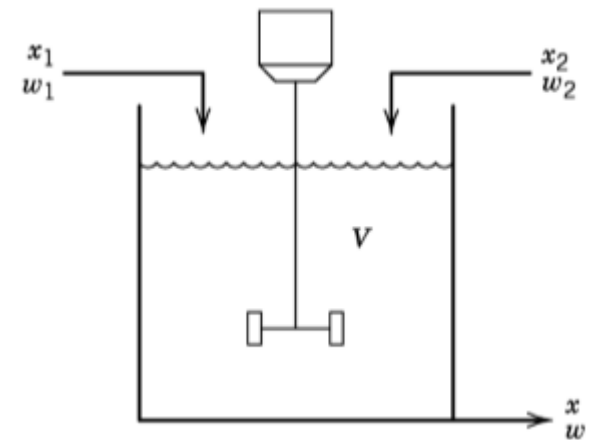
- Dynamic model

- Assumption:  $\rho = \text{constant}$
- From (1) and (2):

$$\rho \frac{dV}{dt} = w_1 + w_2 - w \quad (3)$$

$$\rho \frac{d(Vx)}{dt} = w_1 x_1 + w_2 x_2 - wx \quad (4)$$

## Example: blending process control



- Dynamic model

- Chain rule:

$$\frac{d(Vx)}{dt} = x \frac{dV}{dt} + V \frac{dx}{dt} \quad (5)$$

- From (4) and (5):

$$\rho \frac{d(Vx)}{dt} = \rho x \frac{dV}{dt} + \rho V \frac{dx}{dt} = w_1 x_1 + w_2 x_2 - wx \quad (6)$$

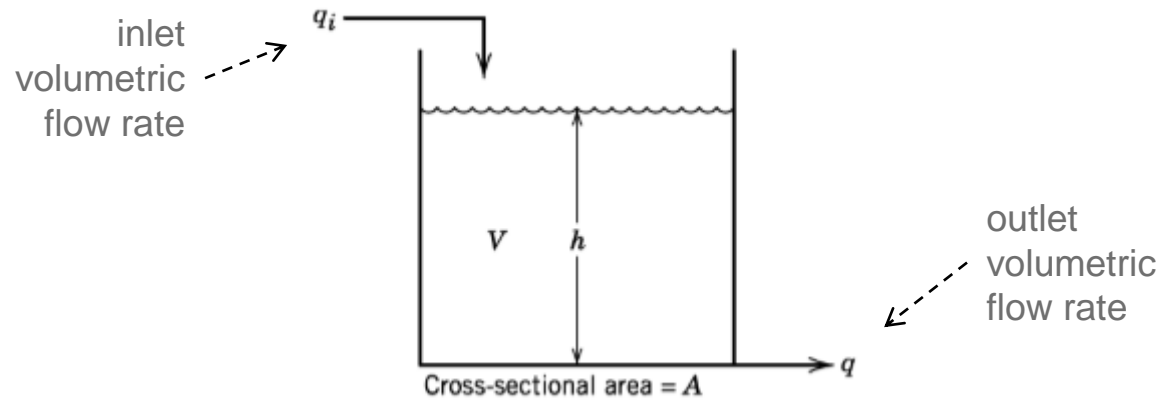
- From (3) and (6):

$$x(w_1 + w_2 - w) + \rho V \frac{dx}{dt} = w_1 x_1 + w_2 x_2 - wx \quad (7)$$

- Dividing (3) and (7) by  $\rho$  and  $\rho V$ , respectively:

$$\begin{cases} \dot{V} = \frac{1}{\rho}(w_1 + w_2 - w) \\ \dot{x} = \frac{w_1}{V\rho}(x_1 - x) + \frac{w_2}{V\rho}(x_2 - x) \end{cases} \quad (8)$$

## Example: liquid storage systems



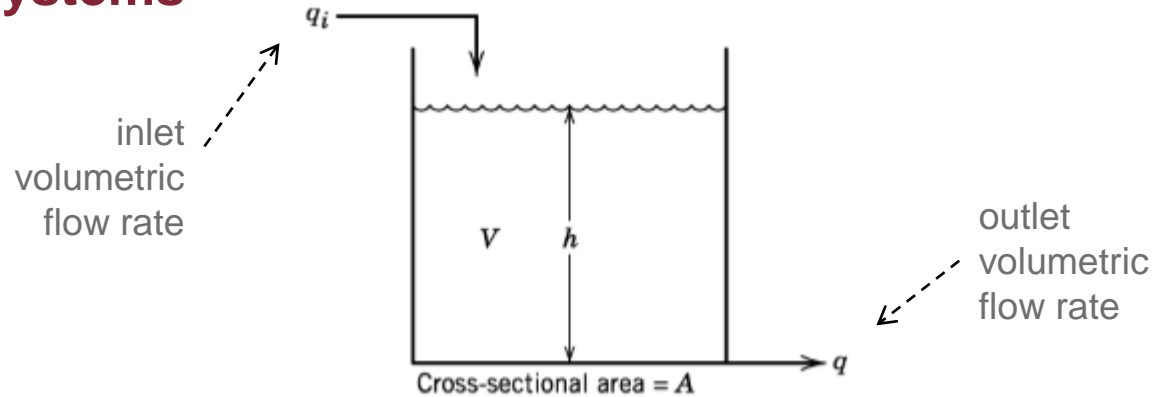
### – Assumptions

- Perfect mixing assumption
- The density  $\rho$  of the liquid is constant
- The tank is cylindrical with area  $A$
- The liquid level is  $h(t)$
- The flow is related to the liquid level

$$h(t) = q(t)R_v$$

where  $R_v$  is the resistance of an outlet valve

## Example: liquid storage systems



- Mass balance

$$\frac{d(\rho V)}{dt} = \rho q_i - \rho q \quad (1)$$

- Volume balance

$$\begin{cases} V = Ah \\ \rho = \text{constant} \end{cases} \Rightarrow A \frac{dh}{dt} = q_i - q \quad (2)$$

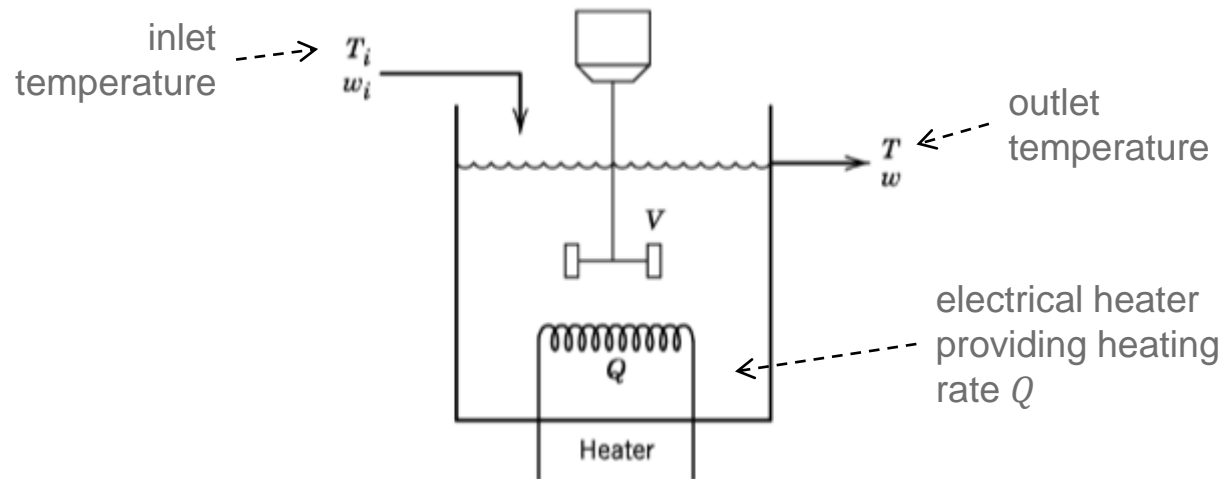
- Assumptions

$$h = q R_v \quad (3)$$

- (2) + (3)

$$\dot{h} = -\frac{1}{AR_v} h + \frac{1}{A} q_i \quad (5)$$

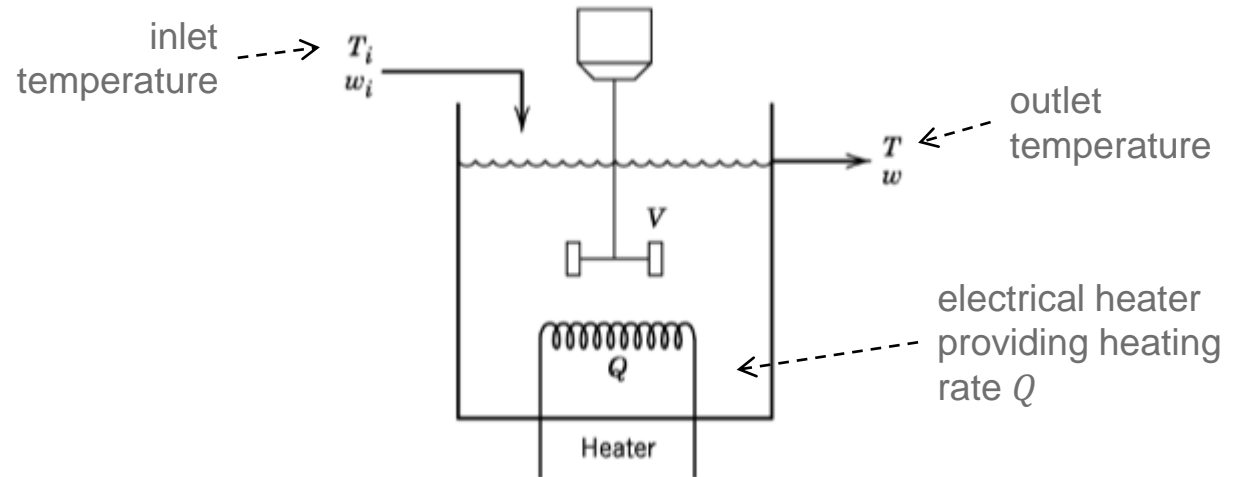
## Example: stirred-tank heating process



### – Assumptions

- Perfect mixing assumption (also the outlet temperature is equal to the one in the tank  $T$ )
- Inlet and outlet flow rates are equal
  - $w_i = w$
  - $V$  is constant
- The density  $\rho$  and the heat capacity  $C$  of the liquid are constant
  - Temperature dependence neglected
- Heat losses are negligible
- The internal energy is equal to the enthalpy  $U_{int} = H$
- $H$  depends only on temperature

## Example: stirred-tank heating process



- Energy balance

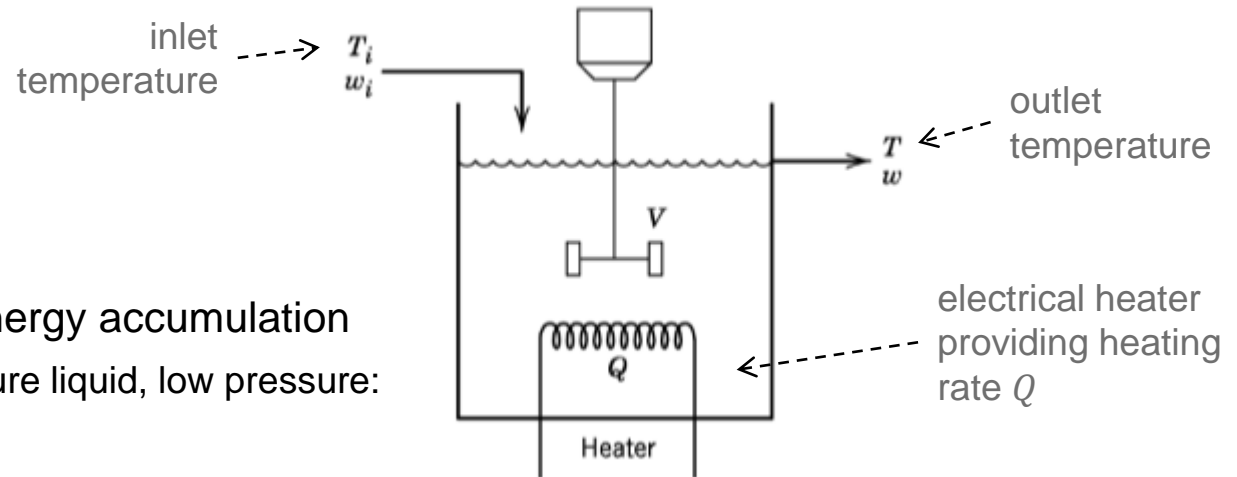
$$\frac{dU_{int}}{dt} = -\Delta(w\hat{H}) + Q$$

where  $\Delta(w\hat{H})$  is the difference of enthalpy between the inlet and the outlet streams

- $\hat{H}$  stands for ‘per unit mass’
- Enthalpy = measurement of energy in a thermodynamic system
- Assumptions: pure liquid, low pressure:
  - 1.  $U_{int} \approx H$
  - 2.  $H$  depends on the temperature only:  $CdT = d\hat{H}$ 
    - where
    - »  $C$  is the pressure heat capacity (assumed constant)
    - »  $dT$  is the change in temperature



## Example: stirred-tank heating process



- Rate of internal energy accumulation
  - Assumptions: pure liquid, low pressure:
    - 1.  $U_{int} \approx H$
    - 2.  $H$  depends on the temperature only

$$CdT = d\hat{H} \quad (1)$$

- »  $C$  is the pressure heat capacity (assumed constant)
- »  $dT$  is the change in temperature

- Total energy in the tank

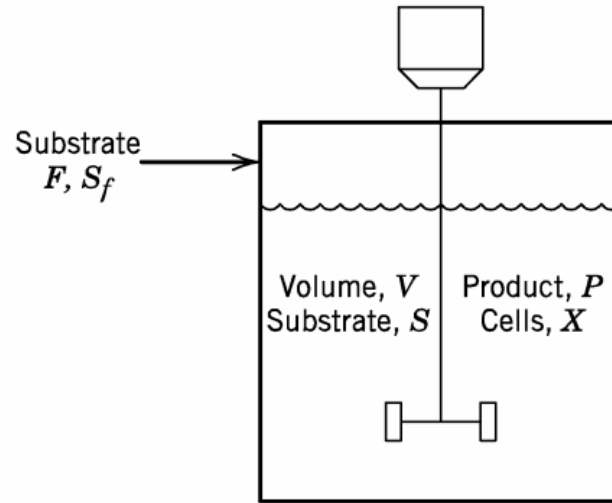
$$U_{int} = \rho V \hat{U}_{int} \quad (2)$$

- (1)+(2)

$$\rho V C \frac{dT}{dt} = \frac{d\hat{U}_{int}}{dT}$$

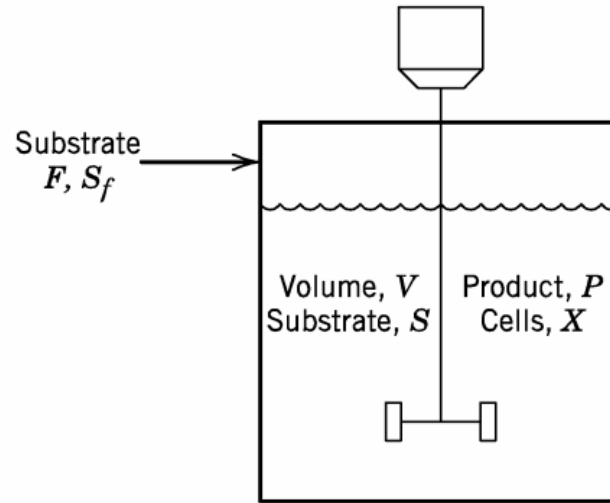
...

## Example: fed-batch (semi-continuous) bioreactor



- Bioreactions
  - Biological reactions that involve microorganisms and enzyme catalysts
  - Basis for production of pharmaceuticals, healthcare and food products
- Simplified law
$$\left\{ \begin{array}{l} \text{feed material} \\ \text{(substrate)} \end{array} \right\} \xrightarrow[\text{(inoculum)}]{\text{cells}} \left\{ \begin{array}{l} \text{cell mass} \\ \text{(biomass)} \end{array} \right\} + \{\text{products}\}$$
- Quantities
  - $F$ : mass flow rate
  - $S_f$ : substrate mass concentration, kept constant (fed-batch)
  - $V$ : volume of the bioreactor content, which increases due to  $F$

## Example: fed-batch (semi-continuous) bioreactor



### – Assumptions

- Cells growth is exponential

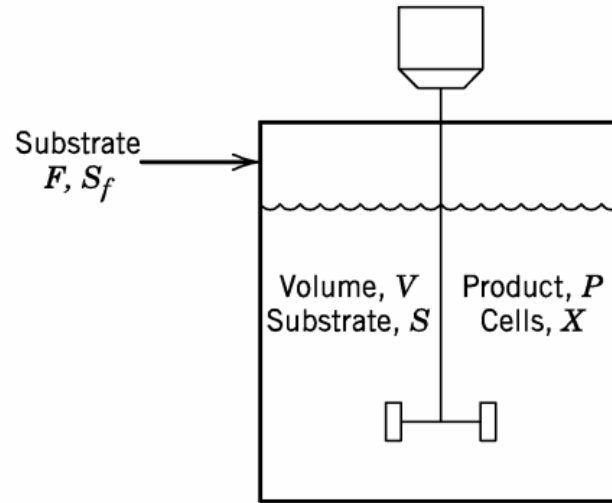
$$r_g = \mu \cdot X$$

- $r_g$ : rate of cell growth per unit volume
- $X$ : cell mass
- $\mu$ : specific growth rate described by the Monod equation [ $t^{-1}$ ]

$$\mu = \mu_{max} \frac{S}{K_S + S}$$

- $K_S$ : Monod constant
- $\mu_{max}$ : maximum growth rate (when  $S \gg K_S$ )

## Example: fed-batch (semi-continuous) bioreactor



### – Assumptions

- Rate of product formation per unit volume

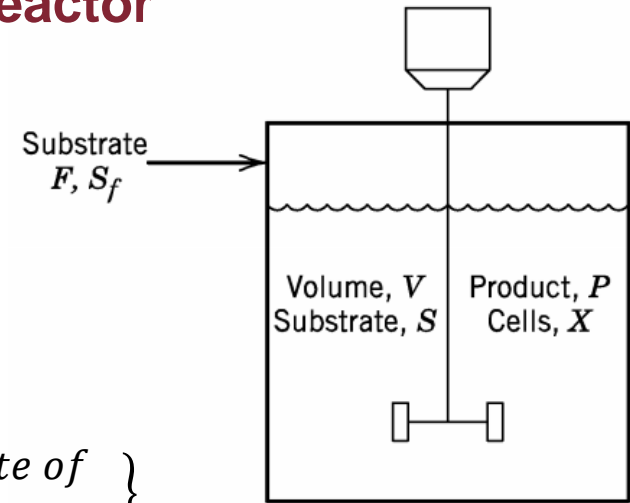
$$r_P = Y_{P/X} \cdot r_g$$

- $r_g$ : rate of cell growth per unit volume
- $Y_{P/X}$ : product yield coefficient

$$Y_{P/X} = \frac{\text{mass of product formed}}{\text{mass of new cells formed}}$$

- Perfect mixing assumption
- Homogeneous liquid assumption
- Heat effect are negligible (isothermal reactor operation)
- The density of the liquid is constant

## Example: fed-batch (semi-continuous) bioreactor



- Balance for substrate, cell, mass, product

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

- Cells balance: 
$$\frac{d(XV)}{dt} = Vr_g$$
- Product balance: 
$$\frac{d(\rho V)}{dt} = Vr_p$$
- Substrate balance: 
$$\frac{d(SV)}{dt} = FS_f - \frac{1}{Y_{X/S}} Vr_g$$
- Overall mass balance, with  $\rho = \text{const.}$ : 
$$\frac{dV}{dt} = F$$

# Linearization of nonlinear models

- Dynamics is generally nonlinear in process models
  - e.g., reaction rate exponential with temperature, pH vs. flow rate of acid or base, ...
- Linearization procedure
  - Given a nonlinear model  $\dot{y}(t) = f(y(t), w(t))$ 
    1. Identify the *operating conditions*
      - The corresponding values of the variables are the *nominal* values, denoted with  $\bar{y}, \bar{w}$
    2. Taylor series expansion at the op. conditions, truncated after the 1st order term

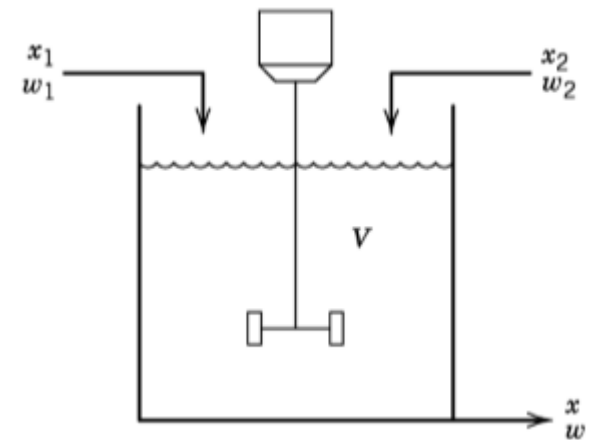
$$\dot{y}(t) = f(y(t), w(t)) \approx f(\bar{y}, \bar{w}) + \left. \frac{\partial f(y, w)}{\partial y} \right|_{\bar{y}, \bar{w}} (y - \bar{y}) + \left. \frac{\partial f(y, w)}{\partial w} \right|_{\bar{y}, \bar{w}} (w - \bar{w})$$

3. Write the equation in terms of the differences with steady-state conditions  $f(\bar{y}, \bar{w}) = 0$

$$\begin{cases} x := y - \bar{y} \\ u := w - \bar{w} \end{cases}$$

$$\dot{x}(t) = \left. \frac{\partial f(y, w)}{\partial y} \right|_{\bar{y}, \bar{w}} x(t) + \left. \frac{\partial f(y, w)}{\partial w} \right|_{\bar{y}, \bar{w}} u(t)$$

# Linearization of nonlinear models



- Blending process control: dynamic model
  - Assuming  $x_2 = 1$ , we obtained a nonlinear model in the state variables  $x, x_1, w_1, w_2$ :

$$\frac{dx(t)}{dt} = \frac{w_1(t)}{V\rho} (x_1(t) - x(t)) + \frac{w_2(t)}{V\rho} (1 - x(t)) = f(x, x_1, w_1, w_2)$$

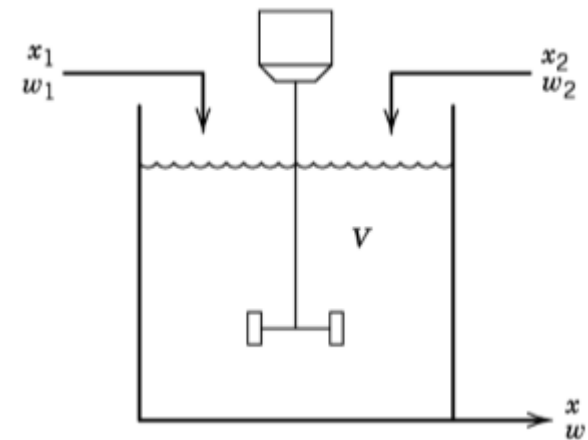
1. Steady state conditions  $(\bar{x}_1, \bar{x}_2 = 1, \bar{w}_1, \bar{w}_2)$ , with  $f(\bar{x}, \bar{x}_1, \bar{w}_1, \bar{w}_2) = 0$

$$\bar{x} = \frac{\bar{w}_1 \bar{x}_1 + \bar{w}_2}{\bar{w}_1 + \bar{w}_2}$$

1. Taylor expansion of  $\frac{dx(t)}{dt} = f(x, x_1, w_1, w_2)$  at the steady-state  $s = (\bar{x}, \bar{x}_1, \bar{w}_1, \bar{w}_2)$

$$\text{in terms of the differences } \begin{cases} x' = x - \bar{x} \\ x'_1 = x_1 - \bar{x}_1 \\ w'_1 = w_1 - \bar{w}_1 \\ w'_2 = w_2 - \bar{w}_2 \end{cases}$$

# Linearization of nonlinear models



- Blending process control: dynamic model

2. Taylor expansion of  $\frac{dx(t)}{dt} = \frac{w_1(t)}{V\rho} (x_1(t) - x(t)) + \frac{w_2(t)}{V\rho} (1 - x(t))$  (cont'd):

$$\frac{dx'(t)}{dt} = \left. \frac{\partial f}{\partial x} \right|_s x'(t) + \left. \frac{\partial f}{\partial x_1} \right|_s x'_1(t) + \left. \frac{\partial f}{\partial w_1} \right|_s w'_1(t) + \left. \frac{\partial f}{\partial w_2} \right|_s w'_2(t)$$

with

$$\left. \frac{\partial f}{\partial x} \right|_s = -\frac{1}{V\rho} (w_1(t) + w_2(t)) \Big|_{(\bar{w}_1, \bar{w}_2)} = -\frac{1}{V\rho} (\bar{w}_1 + \bar{w}_2)$$

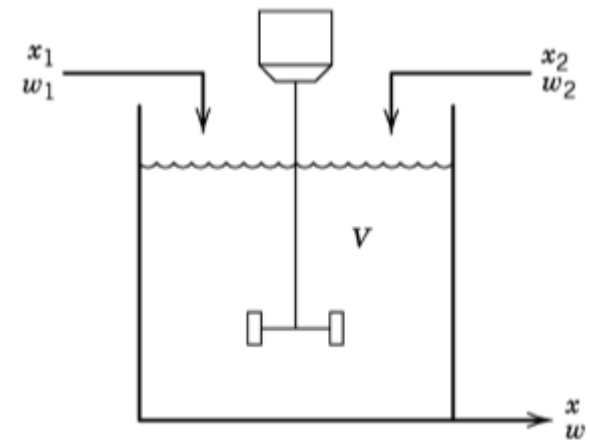
$$\left. \frac{\partial f}{\partial x_1} \right|_s = \frac{1}{V\rho} \bar{w}_1$$

$$\left. \frac{\partial f}{\partial w_1} \right|_s = \frac{1}{V\rho} (\bar{x}_1 - \bar{x})$$

$$\left. \frac{\partial f}{\partial w_2} \right|_s = \frac{1}{V\rho} (1 - \bar{x})$$



# Linearization of nonlinear models



- Blending process control: dynamic model

3. Write the (linear) equation in terms of differences:

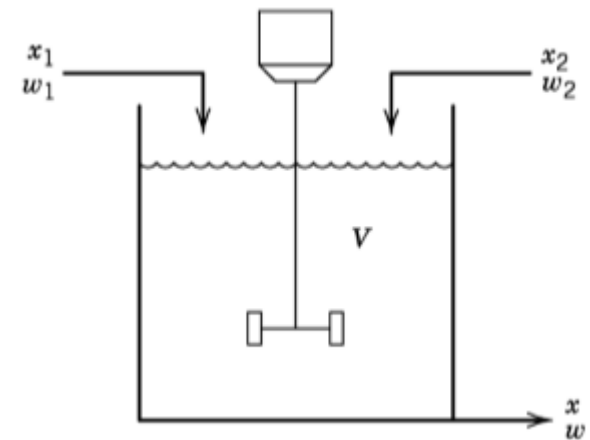
$$\frac{dx'(t)}{dt} = -\frac{1}{V\rho}(\bar{w}_1 + \bar{w}_2)x'(t) + \frac{1}{V\rho}\bar{w}_1x'_1(t) + \frac{1}{V\rho}(\bar{x}_1 - \bar{x})w'_1(t) + \frac{1}{V\rho}(1 - \bar{x})w'_2(t)$$

– Transfer functions

- Laplace transform

$$(sV\rho + (\bar{w}_1 + \bar{w}_2))x'(s) = \bar{w}_1x'_1(s) + (\bar{x}_1 - \bar{x})w'_1(s) + (1 - \bar{x})w'_2(s)$$

# Linearization of nonlinear models



- Blending process control: dynamic model
  - Transfer functions (cont'd)

$$x'(s) = \frac{K_1}{\tau s + 1} x'_1(s) + \frac{K_2}{\tau s + 1} w'_1(s) + \frac{K_3}{\tau s + 1} w'_2(s)$$

where

$$\begin{cases} \tau := \frac{V\rho}{\bar{w}_1 + \bar{w}_2} \\ K_1 := \frac{\bar{w}_1}{\bar{w}_1 + \bar{w}_2} \\ K_2 := \frac{\bar{x}_1 - \bar{x}}{\bar{w}_1 + \bar{w}_2} \\ K_3 := \frac{1 - \bar{x}}{\bar{w}_1 + \bar{w}_2} \end{cases}$$

- Note that the system is externally stable since  $\tau := \frac{V\rho}{\bar{w}_1 + \bar{w}_2} > 0$

# Summary

- Derivation of dynamic models from first principles
- Systematic approach for developing dynamic models
- Examples of process control models referred to continuous processes and batch processes