Introduction

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Introduction

Motivation for Mathematical Modeling

Motivation

- Principles of chemical engineering
  - Perform designed experiments
  - Develop mechanistic understanding
  - Formulate mathematical model
  - Utilize model for system analysis and design
- Mathematical modeling
  - Formal representation of quantitative knowledge
  - Differentiates engineering from discovery science
  - Expertise provides unique professional opportunities
  - Essential component of all ChE courses

The Modeling Process

- Data generation
  - » Experimental design
  - » Data collection and analysis
- Model formulation
  - » Conservation principles and constitutive relations
  - » Parameter estimation and model validation
- Model analysis
  - » Analytical or numerical solution
  - » Qualitative or quantitative analysis
- Model-based design
  - » Chemical reactors (ChE 320)
  - » Fluid systems (ChE 330)
  - » Heat exchangers (ChE 333)
  - » Distillation columns (ChE 338)
  - » Chemical plants (ChE 444)
  - » Control systems (ChE 446)

Classification of Mathematical Models

- Equation type
  - » Algebraic models – no independent variables
  - » ODE models – 1 independent variable
  - » PDE models – 2+ independent variables
- Dimensionality
  - » Low-dimensional model – “small” number of equations
  - » High-dimensional model – “large” number of equations
- Stationarity
  - » Steady-state models – time is not an independent variable
  - » Dynamic models – time is an independent variable

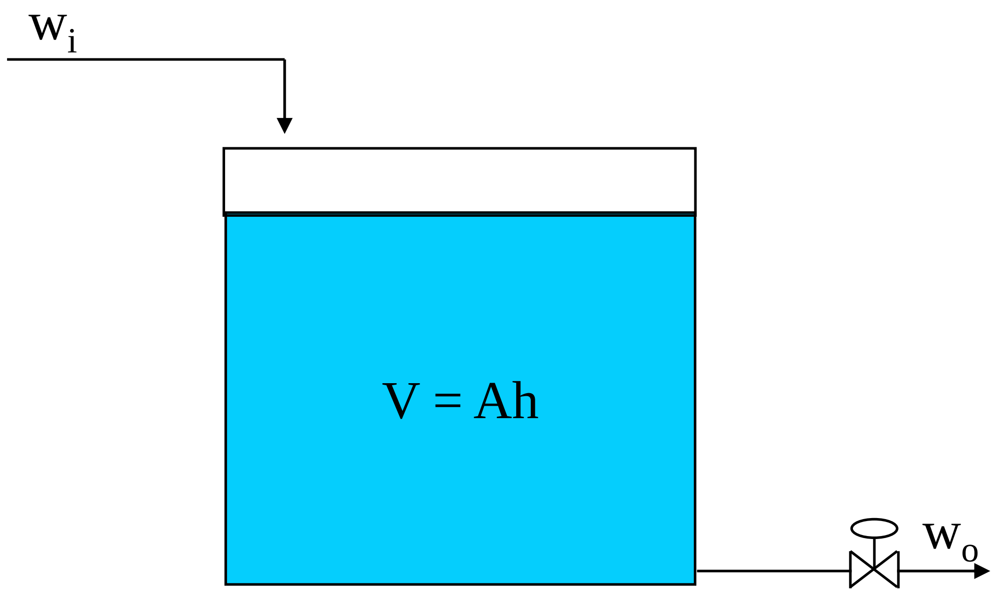
Classification of Mathematical Models

- Linearity
  - » Linear models – all variables appear linearly
  - » Nonlinear models – some variables appear nonlinearly
- Boundary condition type
  - » Initial value problems – boundary conditions specified at one boundary
  - » Mixed boundary value problems – boundary conditions specified at two or more boundaries
- Complexity
  - » Simple – linear, steady-state, low-dimensional, algebraic model
  - » Complex – nonlinear, dynamic, high-dimensional, mixed boundary value, PDE model

Introduction

Illustrative Examples

Liquid Storage Tank



- Linear algebraic model: $0 = w_i - C_v h$
- Nonlinear algebraic model: $0 = w_i - C_v \sqrt{h}$
- Linear ODE model: $\rho A \dfrac{dh}{dt} = w_i - C_v h$
- Nonlinear ODE model: $\rho A \dfrac{dh}{dt} = w_i - C_v \sqrt{h}$

Chemical Reaction Sequence

$$2A + B \xrightarrow{r_1} C \quad A + C \xrightarrow{r_2} D \quad B + 3C \xrightarrow{r_3} D$$

- Reactants A and B supplied at known rates r_{A0} and r_{B0}
- Steady-state mass balances yield system of linear algebraic equations

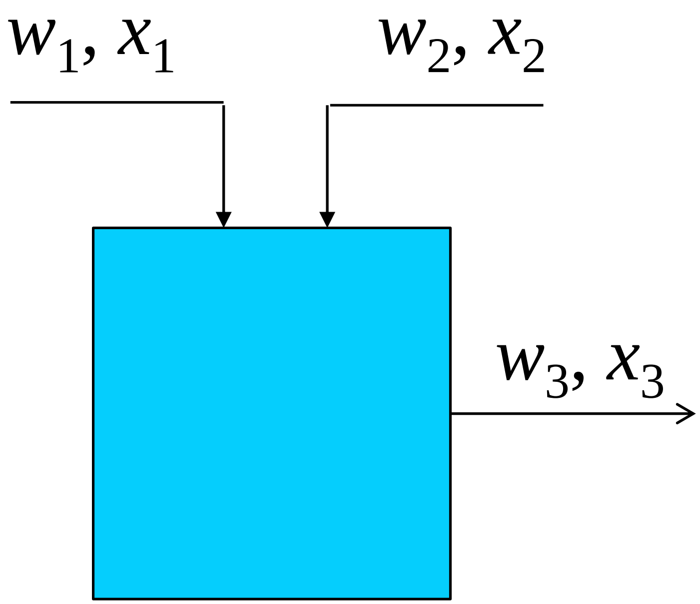
$$\text{A}: \quad 0 = r_{A0} - 2r_1 - r_2$$

$$\text{B}: \quad 0 = r_{B0} - r_1 - r_3$$

$$\text{C}: \quad 0 = r_1 - r_2 - 3r_3$$

- 3 equations and 3 unknowns (r_1, $r_{2,}$,r_3)

Binary Mixing Tank: Steady State

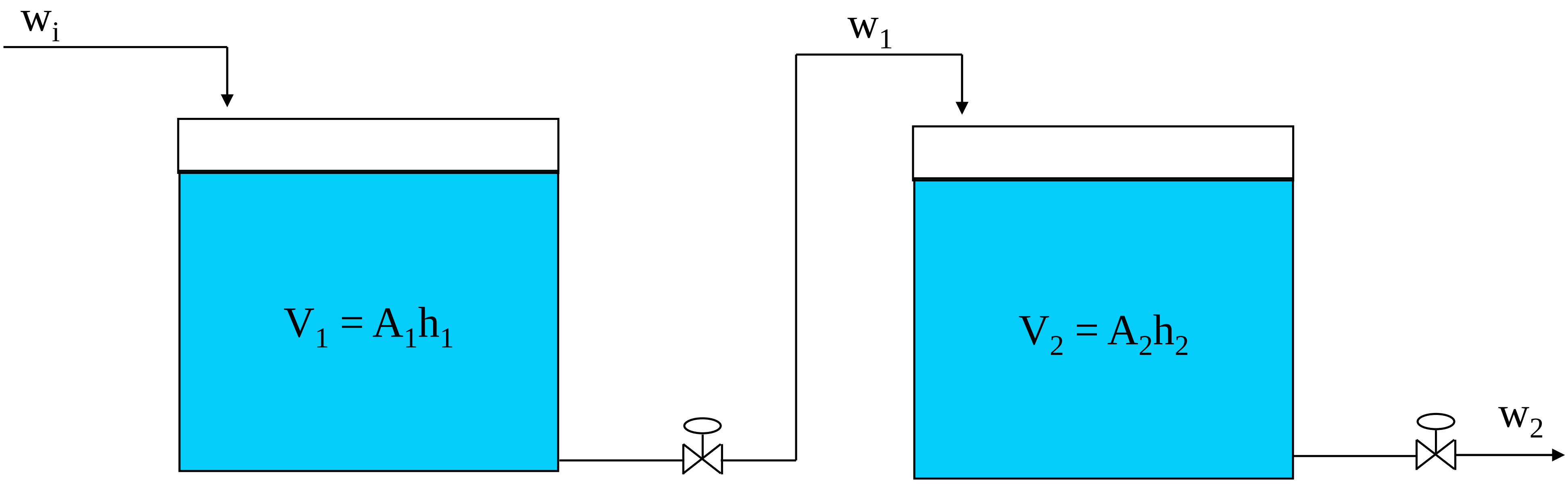


$$0 = w_1 + w_2 - w_3$$

$$0 = w_1 x_1 + w_2 x_2 - w_3 x_3$$

- All inlet stream variable are known (w_1, x_1, w_2, x_2)
- 2 equations with 2 unknowns (w_3, x_3)
- The overall mass balance equation is linear
- The component balance is nonlinear due to $w_3 x_3$ term
- System of nonlinear algebraic equations

Liquid Storage Tanks in Series

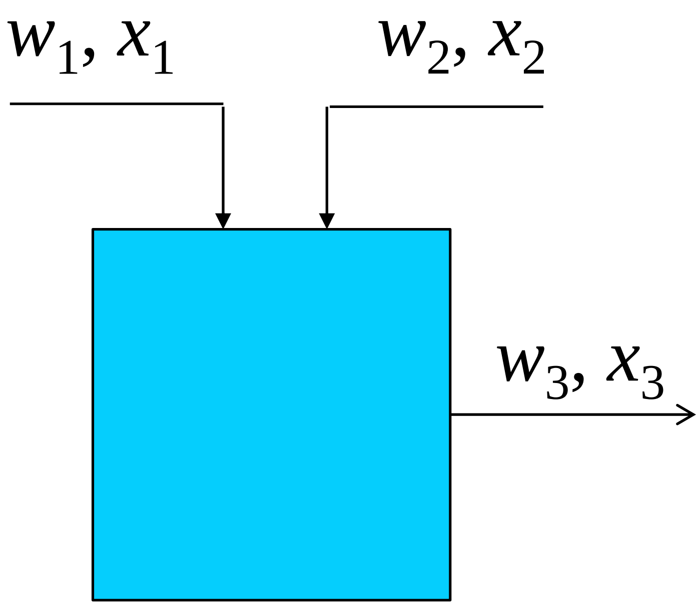


$$\frac{d(\rho A_1 h_1)}{dt} = w_i - C_{v1} h_1$$

$$\frac{d(\rho A_2 h_2)}{dt} = w_1 - C_{v2} h_2 = C_{v1} h_1 - C_{v2} h_2$$

- 2 equations and 2 unknowns (h_1, h_2)
- System of linear ordinary differential equations

Binary Mixing Tank: Unsteady State



$$\frac{d(\rho V)}{dt} = w_1 + w_2 - w_3$$

$$\frac{d(\rho V x_3)}{dt} = w_1 x_1 + w_2 x_2 - w_3 x_3$$

- All inlet stream variable are known (w_1, x_1, w_2, x_2)
- Assume outlet flow rate (w_3) and density (ρ) are known
- 2 equations and 2 unknowns (V, x_3)
- We will learn that both equations are nonlinear
- System of nonlinear ordinary differential equations

Data Analysis: Applied Statistics

Chemical reaction rate data

Experiment	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**
Reactant concentration	0.1	0.3	0.5	0.7	0.9	1.2	1.5	2.0
Reaction rate	2.3	5.7	10.7	13.1	18.5	25.4	32.1	45.2

- Develop a linear model that relates the reactant concentration to the reaction rate

Polymerization reaction rate data

Experiment	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**
Hydrogen concentration	0	0.1	0.3	0.5	1.0	1.5	2.0	3.0
Reaction rate	9.7	9.2	10.7	10.1	10.5	11.2	10.4	10.8

- Determine if the reaction rate is affected by the hydrogen concentration

UMASS.

Introduction

Course Description

Course Description

- Objective
  - » Development and analysis of mathematical models for chemical engineering systems
- Instructor
  - » Prof. Michael A. Henson, N267 Life Science Laboratories, mhenson@umass.edu
- Requirements
  - » Prerequisites: ChE 120
  - » Corequisites: MATH 331 and ChE 226
- Text
  - » E. Kreyzig, Advanced Engineering Mathematics, J. Wiley and Sons, 10th edition (2011).
- Syllabus

Course Objectives

1. Understand the importance of mathematical modeling and analysis in Chemical Engineering.
2. Be able to perform statistical analysis of experimental data and to use computer-based tools for data analysis.
3. Be able to formulate algebraic and ordinary differential models of chemical engineering systems.
4. Be able to solve linear models analytically and to use numerical methods for computer solution of nonlinear models.
5. Develop good engineering practices for composing and solving problems, particularly open-ended problems requiring computer solutions.
6. Be prepared to use the principles and tools learned in this class to solve problems not covered in detail as part of this course and to continue learning related materials as needed in the future.

Schedule

Introduction

In-class Exercise

Quantify Background

- Scoring
  - 5 – I have taken a course that covered the material
  - 4 – I have been substantially exposed to the material
  - 3 – I have been partially exposed to the material
  - 2 – I have been minimally exposed to the material
  - 1 – I have no previous exposure to the material
- Topics
  - Applied statistics
  - Linear algebra
  - Differential equations