Ordinary Differential Equation Models

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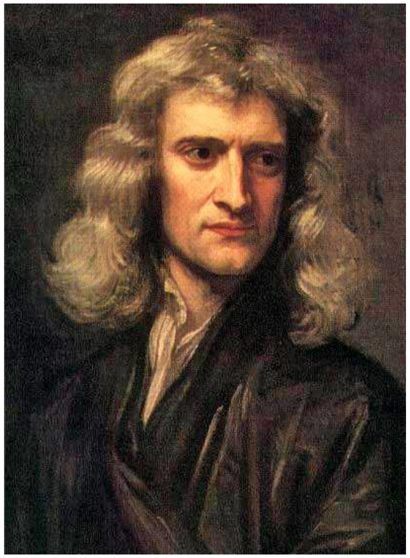

Isaac Newton
1671

Gottfried Wilhelm Leibniz
1675

Jacob Bernoulli
1695

Ordinary Differential Equation Models

Introduction

Motivation

- The modeling process
  - » 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
- Model types
  - » Empirical regression models
  - » Algebraic system models
  - » Ordinary differential equation (ODE) system models
  - » Partial differential equation (PDE) system models

The Modeling Process

- Data generation
  - » Experimental design
  - » Statistical data analysis
- Model formulation
  - » Conservation principles and constitutive relations
  - » Parameter estimation and model validation
- Model analysis
  - » Analytical or numerical solution
  - » Qualitative or quantitative analysis
- Examples of model-based design and analysis
  - » Sizing a chemical reactor to achieve a desired conversion
  - » Determining the number of equilibrium stages in a distillation column to achieve desired product purities
  - » Synthesizing a plant flowsheet with favorable economics
  - » Developing a control system to maintain a process at a desirable steady state

ODE Models

- Ordinary differential equation (ODE) models are ubiquitous throughout chemical engineering
- ODE models are formulated by applying basic conservation laws (mass, energy, momentum, etc.)
- The independent variable can be time or a single spatial coordinate
- ODE models must be solved subject to boundary conditions that are imposed at a particular time or at a particular location in the spatial domain
- Linear ODE models can be solved analytically
- Nonlinear ODE models typically require numerical solution

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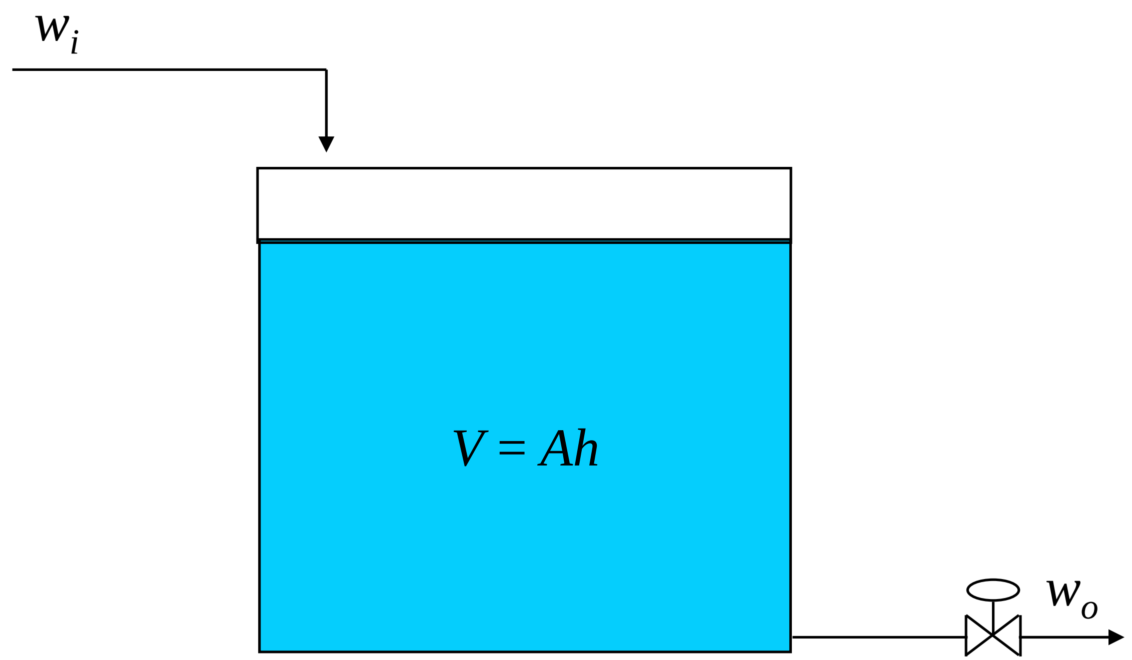
Ordinary Differential Equation Models

Liquid Handling Tanks

Liquid Storage Tank



- Standing assumptions
  - » Constant liquid density ρ
  - » Constant cross-sectional area A
- Other possible assumptions
  - » Steady-state operation
  - » Outlet flow rate w_0 known function of liquid level h

Liquid Storage Tank

- Mass balance on tank:

$$\underbrace{\frac{d(\rho A h)}{dt}}_{\text{accumulation}} = \underbrace{w_i}_{\text{in}} - \underbrace{w_0}_{\text{out}} \quad \Rightarrow \quad \rho A \frac{dh}{dt} = w_i - w_0$$

- Steady-state operation: $0 = \overline{w}_i - \overline{w}_0 \quad \Rightarrow \quad \overline{w}_0 = \overline{w}_i$

- Valve characteristics:

  Linear $\quad w_o = C_v h \quad$ Nonlinear $\quad w_o = C_v \sqrt{h}$

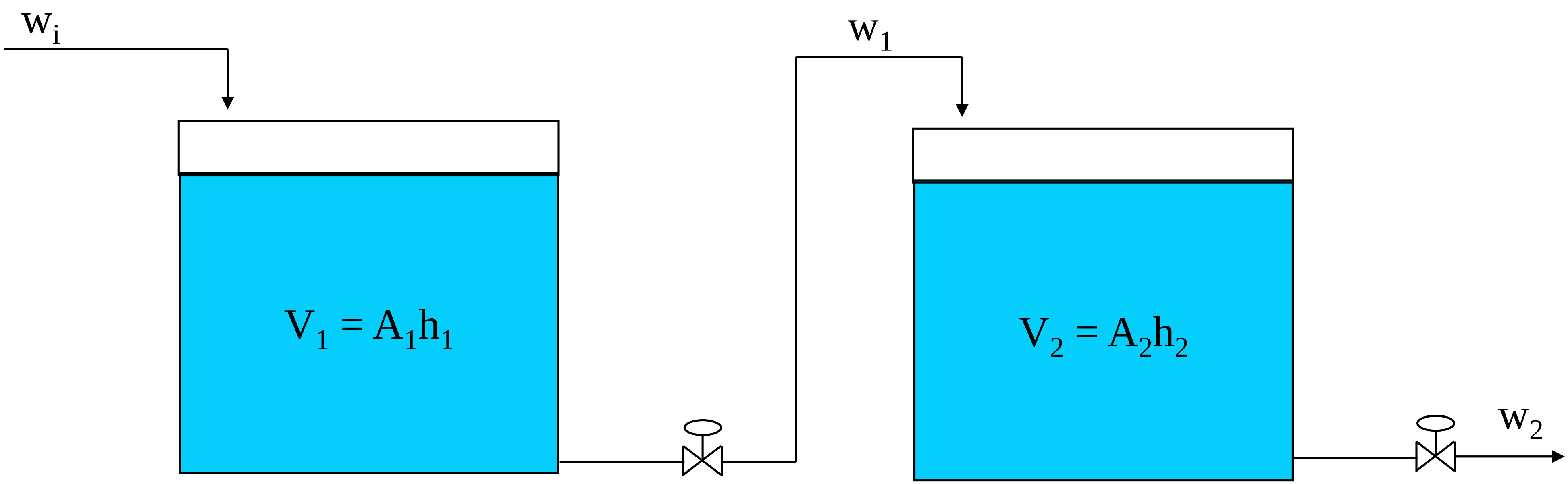
- Linear ODE model:

$$\rho A \frac{dh}{dt} = w_i - C_v h \quad h(0) = h_0$$

- Nonlinear ODE model:

$$\rho A \frac{dh}{dt} = w_i - C_v \sqrt{h} \quad h(0) = h_0$$

Liquid Storage Tanks in Series



- Mass balance on first tank

$$\frac{d(\rho A_1 h_1)}{dt} = w_i - w_1 = w_i - C_{v1} h_1$$

$$\frac{dh_1}{dt} = \frac{w_i - C_{v1} h_1}{\rho A_1} \qquad h_1(0) = h_{10}$$

Liquid Storage Tanks in Series

- Mass balance on second tank

$$\frac{d(\rho A_2 h_2)}{dt} = w_1 - w_2 = C_{v1}h_1 - C_{v2}h_2$$

$$\frac{dh_2}{dt} = \frac{C_{v1}h_1 - C_{v2}h_2}{\rho A_2} \qquad h_2(0) = h_{20}$$

- Linear ODE system

$$\frac{dh_1}{dt} = \frac{w_i - C_{v1}h_1}{\rho A_1} \qquad h_1(0) = h_{10}$$

$$\frac{dh_2}{dt} = \frac{C_{v1}h_1 - C_{v2}h}{\rho A_2} \qquad h_2(0) = h_{20}$$

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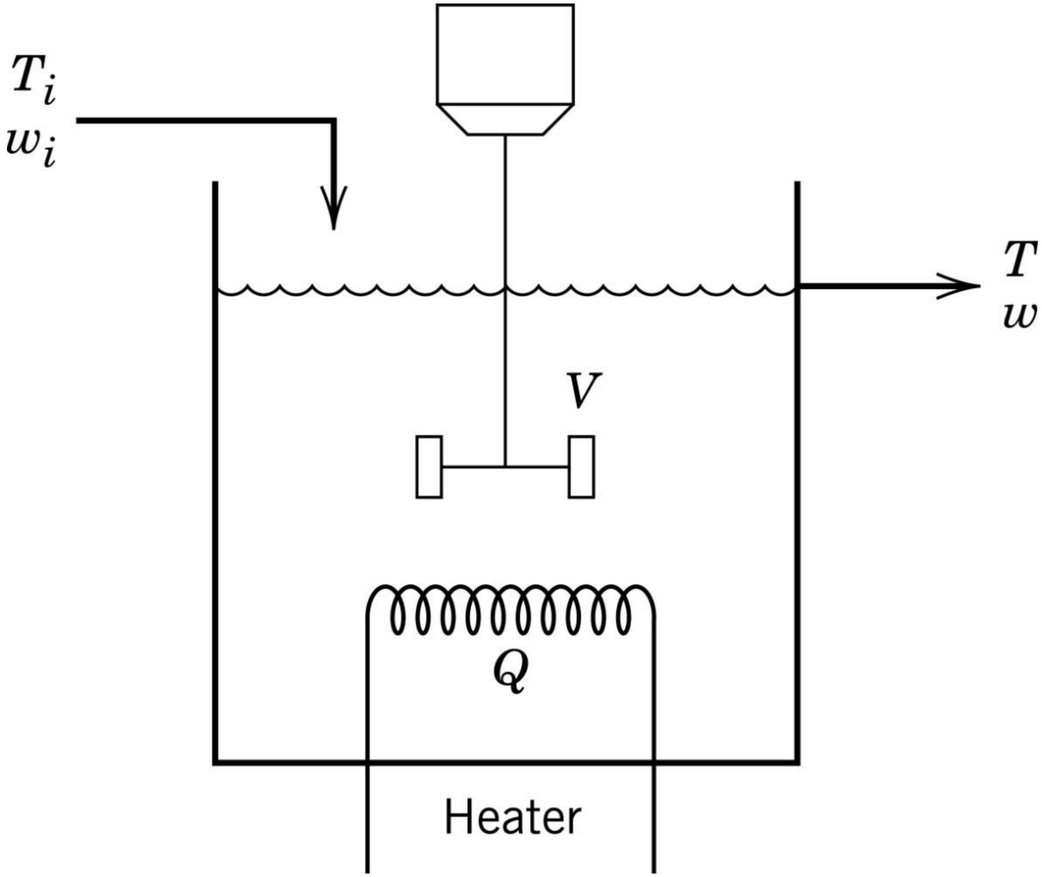
Continuous Stirred Tank Heater



Assumptions:

- Constant volume
- Perfect mixing
- Negligible heat losses
- Constant physical properties (ρ, C_p)

Continuous Stirred Tank Heater

- Mass balance

$$\frac{d(\rho V)}{dt} = 0 = w_i - w \quad \Rightarrow \quad w_i = w$$

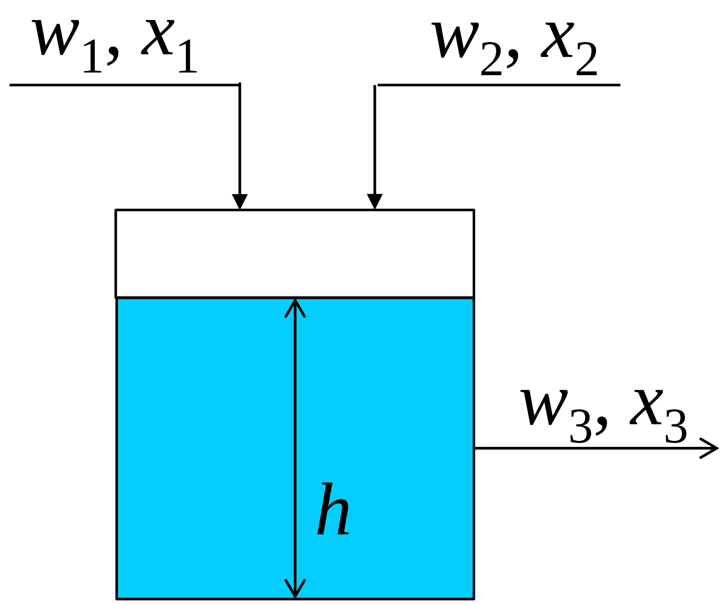
- Energy balance

$$\frac{d}{dt}\left[\rho V C_p (T - T_{ref})\right] = w_i C_p (T_i - T_{ref}) - w C_p (T - T_{ref}) + Q$$

$$\rho V C_p \frac{dT}{dt} = w C_p (T_i - T) + Q$$

$$\frac{dT}{dt} = \frac{w C_p (T_i - T) + Q}{\rho V C_p} \quad T(0) = T_0$$

Binary Mixing Tank



Key assumption:
the tank is perfectly mixed

- Overall mass balance:

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

$$\frac{dh}{dt} = \frac{w_1 + w_2 - w_3}{\rho A} \qquad h(0) = h_0$$

Binary Mixing Tank

- Component balance

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

$$\frac{d(\rho V x_3)}{dt} = \rho V \frac{dx_3}{dt} + x_3 \frac{d(\rho V)}{dt} = \rho V \frac{dx_3}{dt} + x_3 (w_1 + w_2 - w_3)$$

$$\rho V \frac{dx_3}{dt} + x_3 (w_1 + w_2 - w_3) = w_1 x_1 + w_2 x_2 - w_3 x_3$$

$$\frac{dx_3}{dt} = \frac{w_1 (x_1 - x_3) + w_2 (x_2 - x_3)}{\rho A h} \qquad x_3(0) = x_{30}$$

Binary Mixing Tank

- Nonlinear ODE system:

$$\frac{dh}{dt} = \frac{w_1 + w_2 - w_3}{\rho A} \qquad h(0) = h_0$$

$$\frac{dx_3}{dt} = \frac{w_1(x_1 - x_3) + w_2(x_2 - x_3)}{\rho A h} \qquad x_3(0) = x_{30}$$

- 2 equations and 2 unknowns (h, x_3)
- The ODEs are coupled through the variable h
- Solution: $h(t)$, $w_3(t)$

Ordinary Differential Equation Models

In-class Exercise

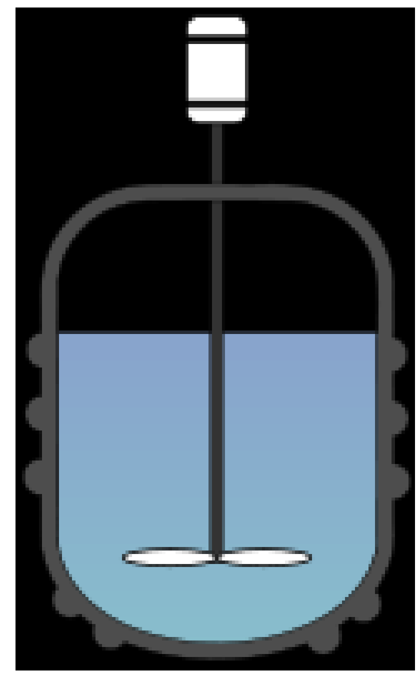
Ordinary Differential Equation Models

Chemical Reactors

Batch Chemical Reactor

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

- The reactor is charged with reactants A and B at concentrations C_{A0} and C_{B0} at time $t = 0$
- The reaction proceeds until some final time $t = t_f$
- The reactor has constant liquid volume V
- The reaction rates per unit volume of liquid are:



$$r_1 = k_1 C_A^2 C_B \quad r_2 = k_2 C_A C_C \quad r_3 = k_3 C_B C_C^3$$

Batch Chemical Reactor

- Overall mass balance:

$$\frac{d(\rho V)}{dt} = 0 \quad \Rightarrow \quad V(t) = V$$

- Component balances:

$$\frac{d(VC_A)}{dt} = -2r_1 - r_2 = -2k_1 C_A^2 C_B V - k_2 C_A C_C V$$

$$\frac{d(VC_B)}{dt} = -r_1 - r_3 = -k_1 C_A^2 C_B V - k_3 C_B C_C^3 V$$

$$\frac{d(VC_C)}{dt} = r_1 - r_2 - 3r_3 = k_1 C_A^2 C_B V - k_2 C_A C_C V - 3k_3 C_B C_C^3 V$$

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Batch Chemical Reactor

- Nonlinear ODE system:

$$\frac{dC_A}{dt} = -2k_1 C_A^2 C_B - k_2 C_A C_C \qquad C_A(0) = C_{A0}$$

$$\frac{dC_B}{dt} = -k_1 C_A^2 C_B - k_3 C_B C_C^3 \qquad C_B(0) = C_{B0}$$

$$\frac{dC_C}{dt} = k_1 C_A^2 C_B - k_2 C_A C_C - 3k_3 C_B C_C^3 \qquad C_C(0) = 0$$

- 3 equations and 3 unknowns (C_A, C_B, C_C)
- The ODEs are fully coupled
- Solution: $C_A(t)$, $C_B(t)$, $C_C(t)$

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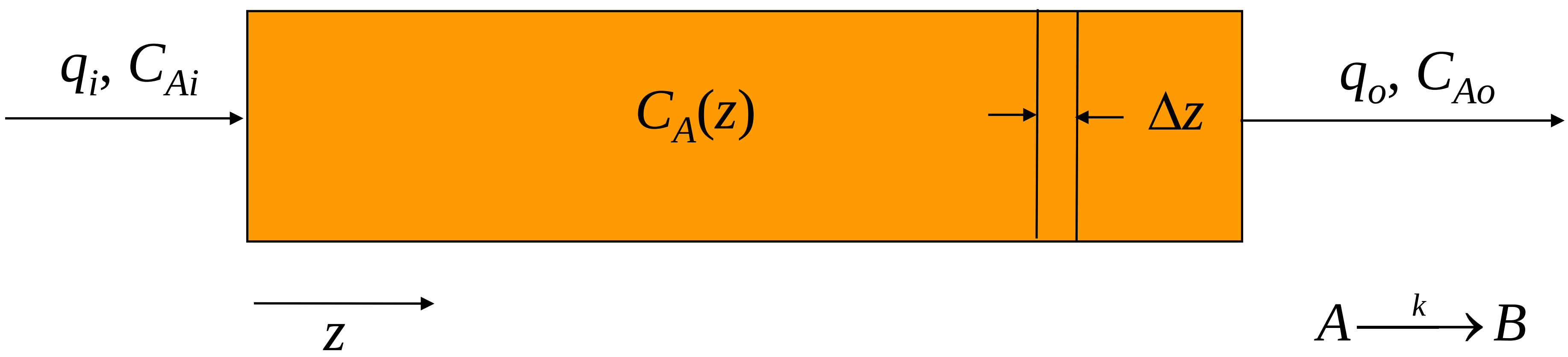
Plug-Flow Chemical Reactor

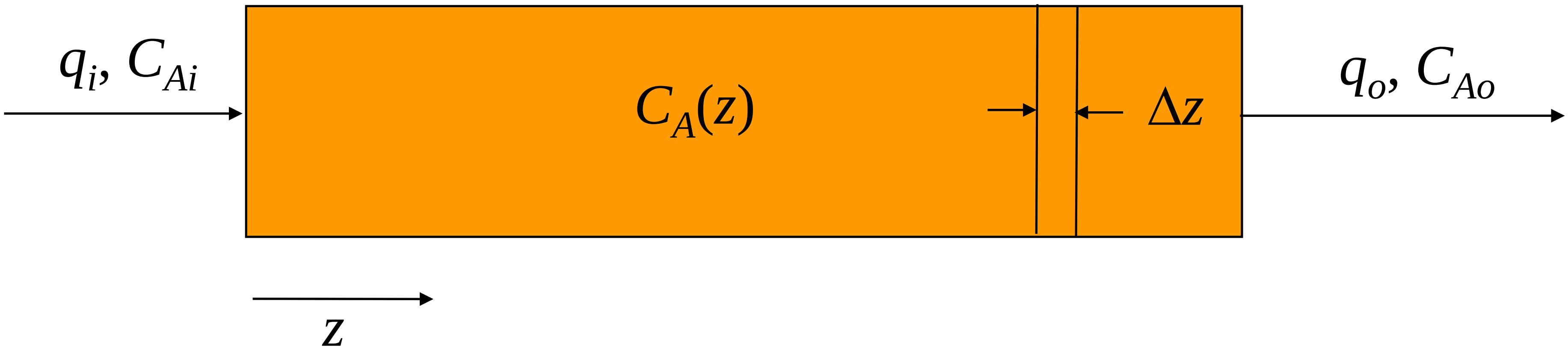


$$A \xrightarrow{k} B$$

$$r = kC_A$$

- Assumptions
  - » Pure reactant A in feed stream
  - » Steady-state operation
  - » Isothermal operation
  - » Constant physical properties (ρ, k)

Plug-Flow Chemical Reactor



- Overall mass balance:

$$\underbrace{(\rho q)_z}_{\text{Mass in}} - \underbrace{(\rho q)_{z+\Delta z}}_{\text{Mass out}} = 0$$

$$\lim_{\Delta z \to 0}\left[\frac{(q)_z - (q)_{z+\Delta z}}{\Delta z}\right] = 0$$

$$-\frac{dq}{dz} = 0 \qquad \Rightarrow \qquad q_i = q_0 = q$$

Plug-Flow Chemical Reactor

- Component balance:

$$\underbrace{(qC_A)_z}_{\text{A in}} - \underbrace{(qC_A)_{z+\Delta z}}_{\text{A out}} - \underbrace{kC_A A\Delta z}_{\text{A consumed}} = 0$$

$$\lim_{\Delta z \to 0}\left[\frac{q}{A}\frac{(C_A)_z - (C_A)_{z+\Delta z}}{\Delta z} - kC_A\right] = 0$$

$$-\frac{q}{A}\frac{dC_A}{dz} - kC_A = 0$$

$$\frac{q}{A}\frac{dC_A}{dz} + kC_A = 0 \quad C_A(0) = C_{Ai}$$

- Solution: $C_A(z)$