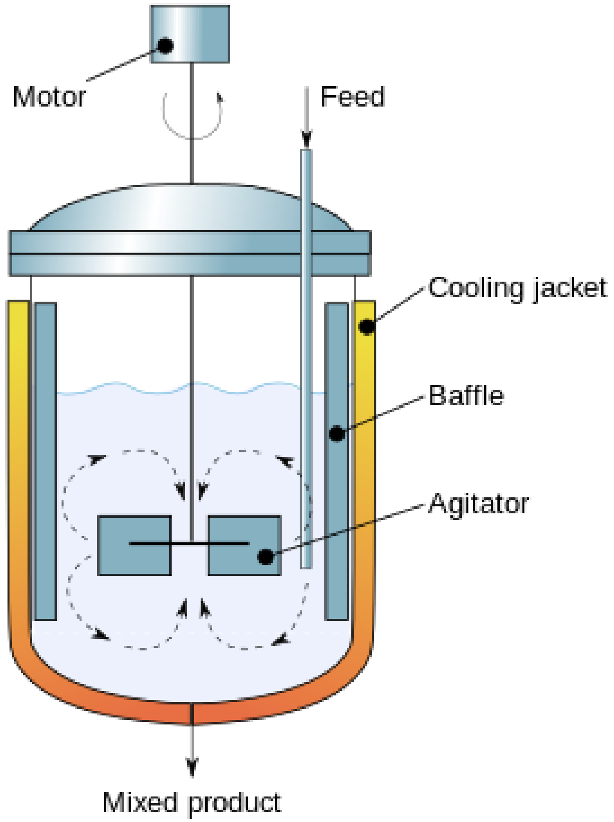
DYNAMIC BALANCES

Modeling fundamental chemical engineering units



UNIVERSITY OF WATERLOO

LEARNING OUTCOMES

- Derive 1st principles equations for dynamic chemical engineering units based on balance equations
- Identify and label the inputs and ouputs

RESOURCES

- Video lectures, notes, and examples
  - https://apmonitor.com/pdc/index.php/Main/PhysicsBasedModels
  - https://apmonitor.com/pdc/index.php/Main/DynamicModeling

GENERAL BALANCE EQUATION

- The bread and butter of chemical engineering

$$accumulation = in - out + generation - consumption$$

- Our focus will be on transient systems ($accumulation \neq 0$)
- Typically, four quantities are conserved
  - Mass
  - Species
  - Momentum
  - Energy

MASS BALANCE

- General equation

$$\frac{dm}{dt} = \frac{d(\rho V)}{dt} = \sum \dot{m}_{in} - \sum \dot{m}_{out}$$

- If all densities are constant and equal

$$\frac{dV}{dt} = \sum \dot{V}_{in} - \sum \dot{V}_{out}$$

SPECIES (MOLAR) BALANCE

- Track number of species n_A (in moles) with respect to a prescribed space

$$\frac{dn_A}{dt} = \sum \dot{n}_{A_{in}} - \sum \dot{n}_{A_{out}} + \sum \dot{n}_{A_{gen}} - \sum \dot{n}_{A_{cons}}$$

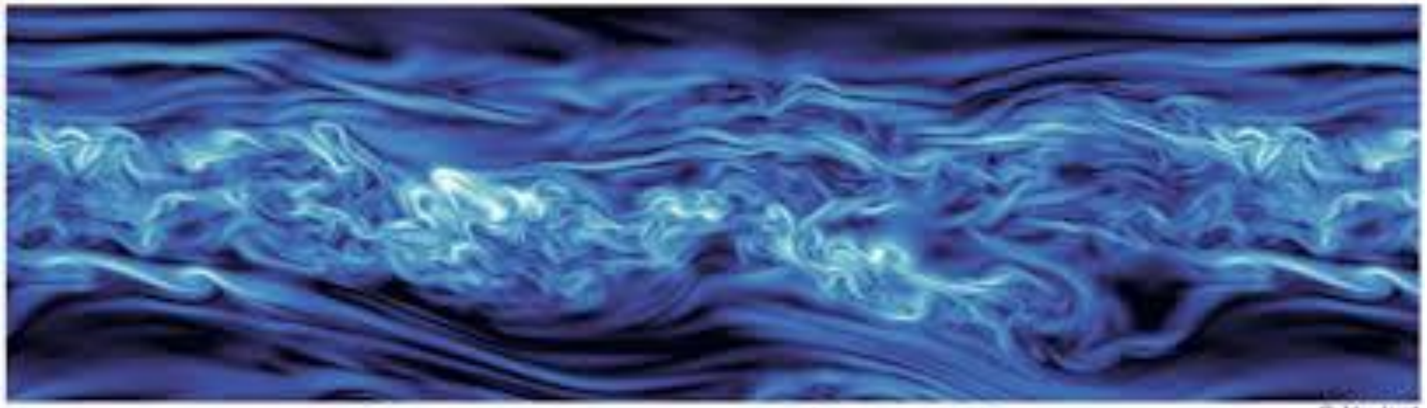
- Often reformulate in terms of concentration c_A and reaction rate r_A
  - Reaction rate is net molar generation per unit volume

$$\frac{dc_A V}{dt} = \sum c_{A_{in}} \dot{V}_{in} - \sum c_{A_{out}} \dot{V}_{out} + r_A V$$

MOMENTUM BALANCE

- The accumulation of momentum is equal to the sum of the forces F

$$\frac{d(m\,v)}{dt} = \sum F$$



ENERGY BALANCE

- General equation
$$\frac{dE}{dt} = \frac{d(U + \cancel{K} + \cancel{P})}{dt} = \sum \dot{m}_{in} \left(\hat{h}_{in} + \cancel{\frac{v_{in}^2}{2g_c}} + \cancel{\frac{z_{in} g_{in}}{g_c}} \right)$$
$$- \sum \dot{m}_{out} \left(\hat{h}_{out} + \cancel{\frac{v_{out}^2}{2g_c}} + \cancel{\frac{z_{out} g_{out}}{g_c}} \right) + Q + W_s$$

- For most chemical processes, the kinetic and potential terms K and P are negligible relative to the energy changes driven by temperature
$$\frac{dh}{dt} = \sum \dot{m}_{in} \hat{h}_{in} - \sum \dot{m}_{out} \hat{h}_{out} + Q + W_s$$

- Use the relation h = $mc_p(T - T_{ref})$ (assumes constant heat capacity and mass)
$$m\, c_p \frac{dT}{dt} = \sum \dot{m}_{in} c_p \left(T_{in} - T_{ref} \right) - \sum \dot{m}_{out} c_p \left(T_{out} - T_{ref} \right) + Q + W_s$$

DYNAMIC MODELING RECIPE

1. Identify objective for the simulation
2. Draw a schematic diagram, labeling process variables
3. List all assumptions
4. Determine spatial dependence
    - yes = Partial Differential Equation (PDE)
    - no = Ordinary Differential Equation (ODE)
5. Write dynamic balances (mass, species, energy)
6. Other relations (thermo, reactions, geometry, etc.)
7. Degrees of freedom, does number of equations = number of unknowns?

DYNAMIC MODELING RECIPE (CONTINUED)

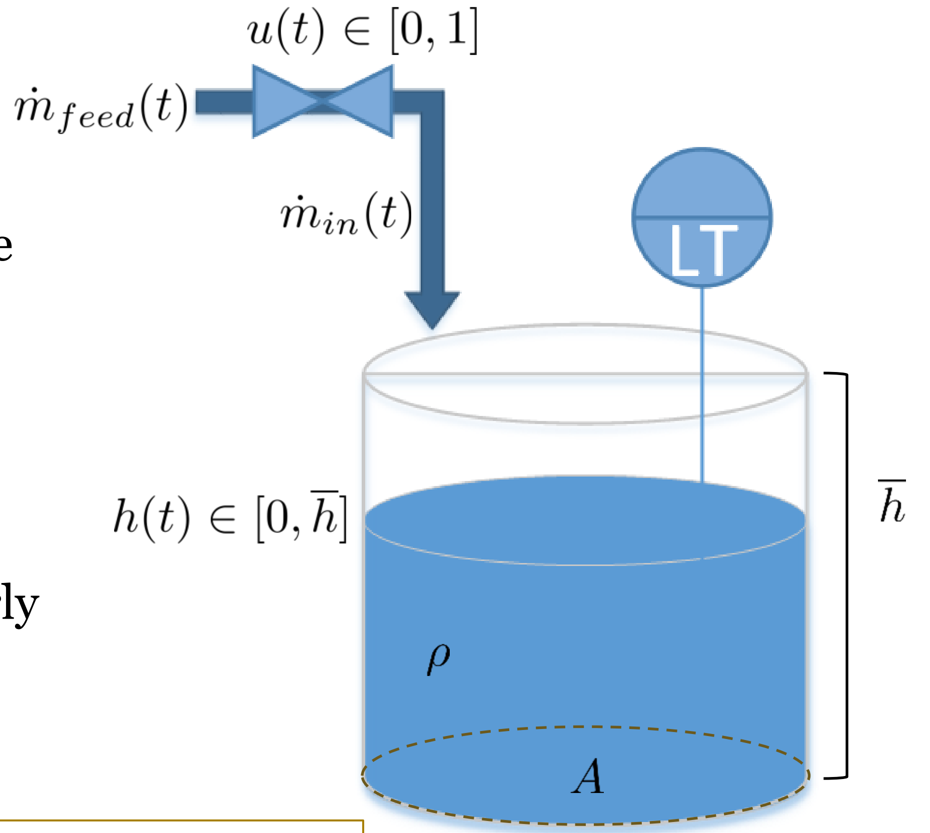
8. Classify inputs as
   - Fixed values
   - Disturbances
   - Manipulated variables
9. Classify outputs as
   - States
   - Controlled variables
10. Simplify balance equations based on assumptions
11. Simulate steady state conditions (if possible)
12. Simulate the output with an input step

EXAMPLE: FILLING A WATER TANK

- Develop a model that can maintain a certain water level by automatically adjusting the inlet flow rate.
- Consider a cylindrical tank with no outlet flow and an adjustable inlet flow. The inlet flow rate is not measured but the level is.

1. *Objective:* Determine how tank level changes in valve position
2. *Schematic with variables*
3. *Assumptions:* Constant density ρ, inlet flow rate changes linearly with valve position, cross-sectional area is constant
4. *Spatial dependence?:* None
5. *Write balances*

$$\frac{dm}{dt} = \dot{m}_{in} - \cancel{\dot{m}_{out}} + \cancel{\dot{m}_{gen}}$$



Note: Reading material uses units of % open instead of fraction open.

Note: Reading material doesn't treat $\dot{m}_{feed}$ as a variable.

EXAMPLE: FILLING A WATER TANK

6. *Other relations*

$$\dot{m}_{in} = u \cdot \dot{m}_{feed} \qquad m = \rho V = \rho A h$$

7. *Degrees of freedom:* 5 variables ($\dot{m}_{feed}, u, \dot{m}_{in}, m, h$), 3 equations → 2 DoF

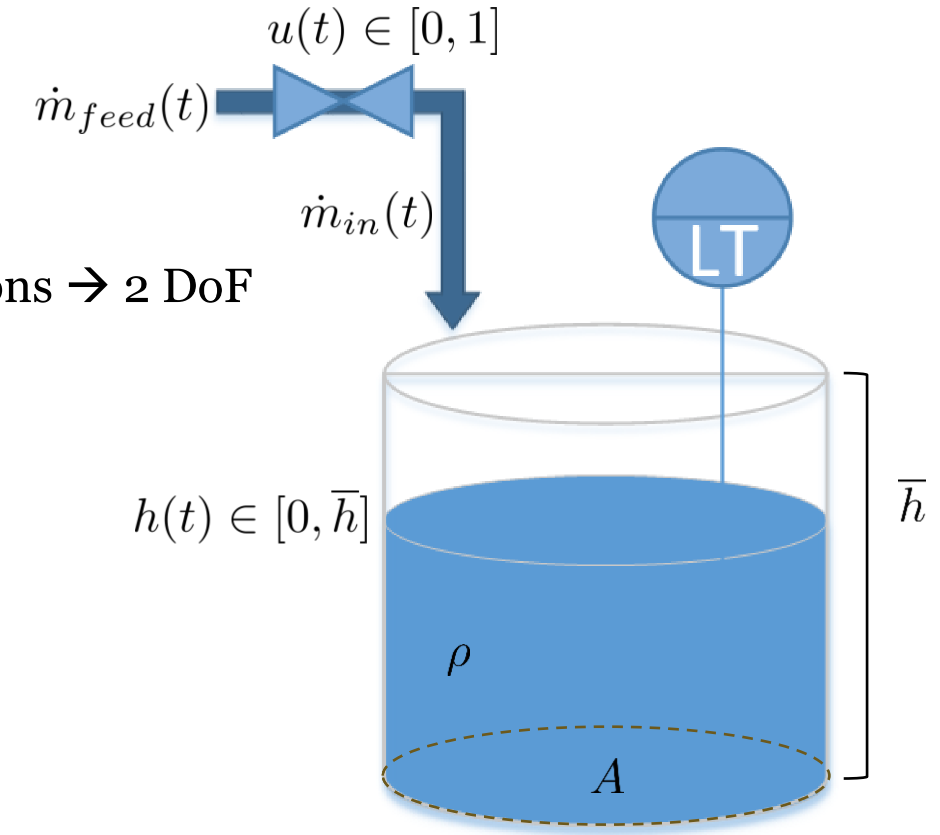
8. *Classify inputs:* $\dot{m}_{feed}$ (disturbance), u (manipulated)

9. *Classify outputs:* $\dot{m}_{in}$ (state), h (controlled), m (state)

10. *Simplify balances*

$$\frac{dm}{dt} = \dot{m}_{in} \quad \Rightarrow \quad \rho A \frac{dh}{dt} = u \cdot \dot{m}_{feed}$$

11. *Steady state:* Trivially, the height stays constant



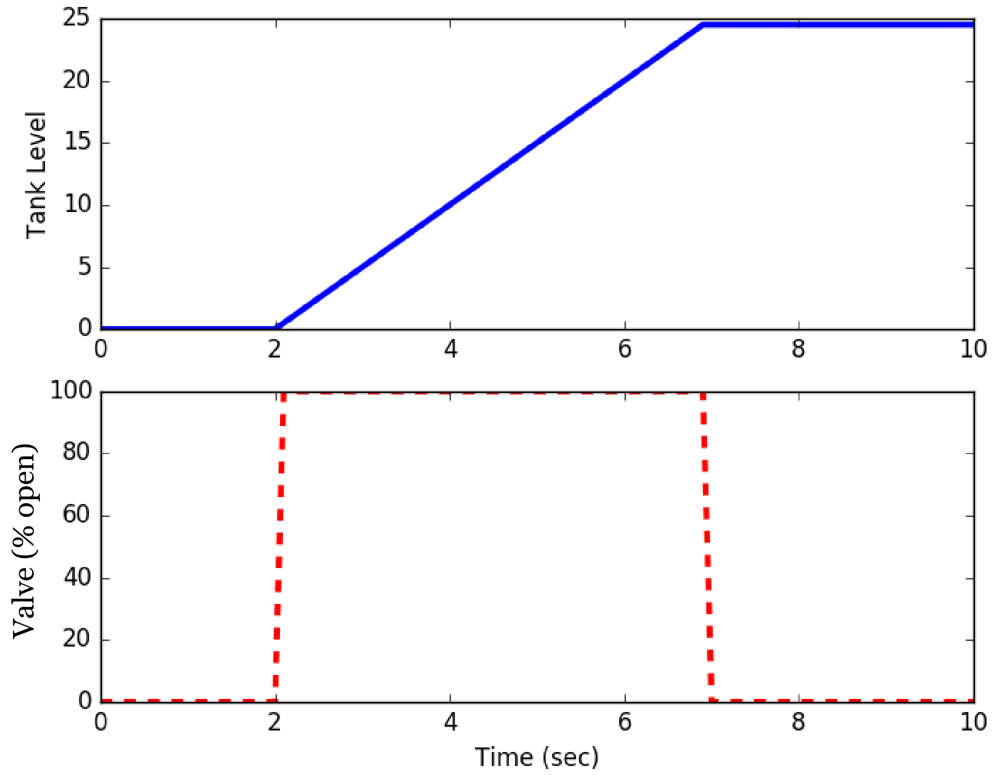
Note: Reading material uses a slightly different valve equation.

EXAMPLE: FILLING A WATER TANK

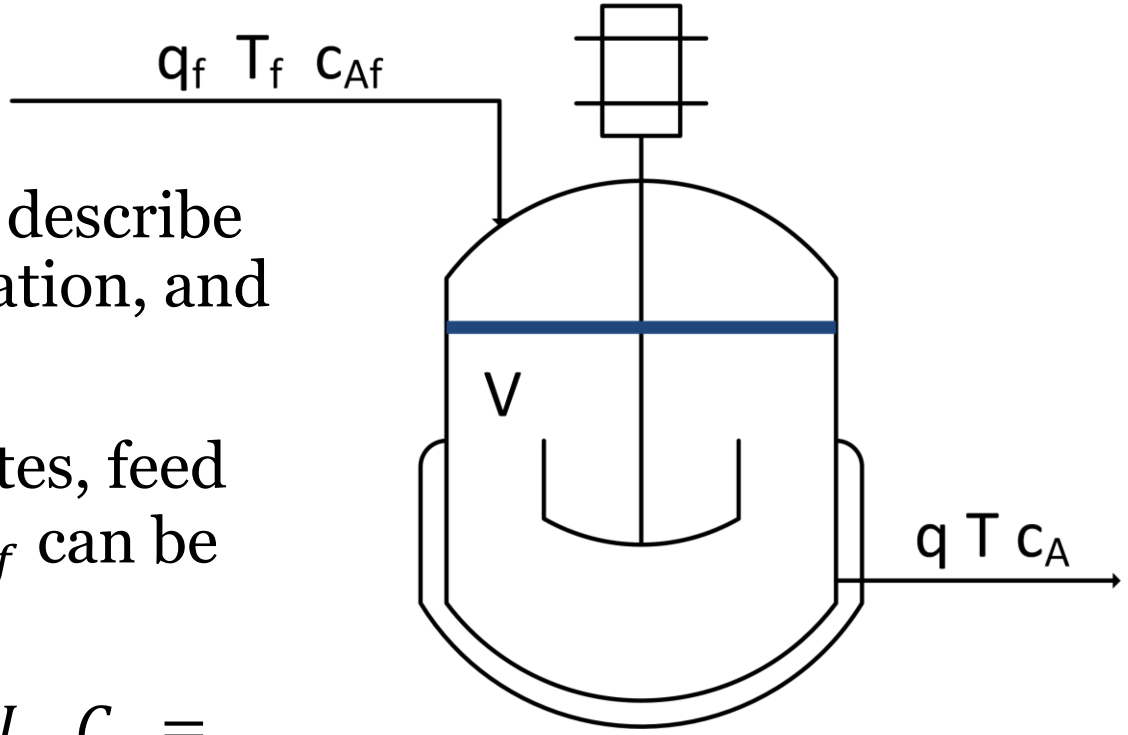
12. *Dynamic response*

- $u(t) := \begin{cases} 1, & 2 \le t \le 7 \\ 0, & otherwise \end{cases}$
- $\dot{m}_{feed}(t) = 50\frac{kg}{s}$
- $\rho = 1000\frac{kg}{m^3}$
- $A = 1.0m^2$

$$\rho A \frac{dh}{dt} = u \cdot \dot{m}_{feed}$$

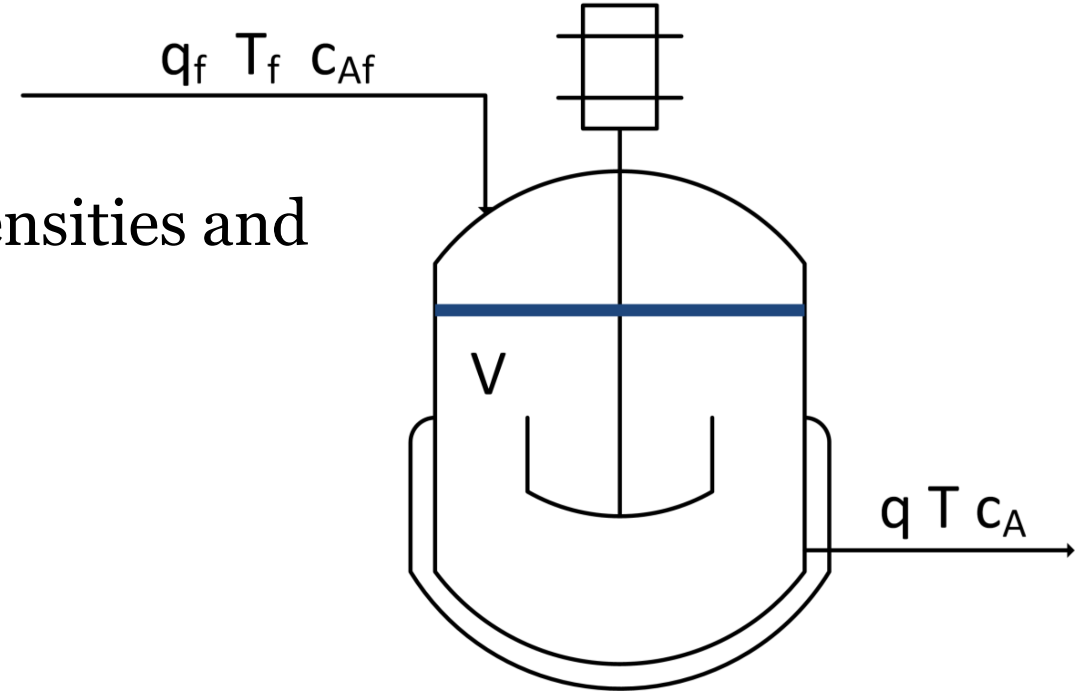


CASE STUDY: DYNAMIC MIXER



- Use a mass, species, and energy balance to describe the dynamic response in volume, concentration, and temperature of a well-mixed vessel.
- The inlet q_f and outlet q volumetric flowrates, feed concentration C_{af}, and inlet temperature T_f can be adjusted
- Initial conditions for the vessel are $V = 1.0L,\ C_a = 0.0\frac{mol}{L}, T = 350K.$
- There is no reaction and no significant heat added by the mixer.

CASE STUDY: DYNAMIC MIXER



3. *Assumptions:* No rxn, no heat added, all densities and heat capacities are uniform and constant
4. *Spatial dependence:* None
5. *Balances:*
   - *Mass balance*

$$\rho\frac{dV}{dt} = \rho q_f - \rho q \quad \xrightarrow{\text{Constant and equal densities}} \quad \frac{dV}{dt} = q_f - q$$

CASE STUDY: DYNAMIC MIXER

5. Balances

- Species balance

No rxn

$$\frac{d(c_A V)}{dt} = c_{Af} q_f - c_A q + \cancel{r_A} V$$

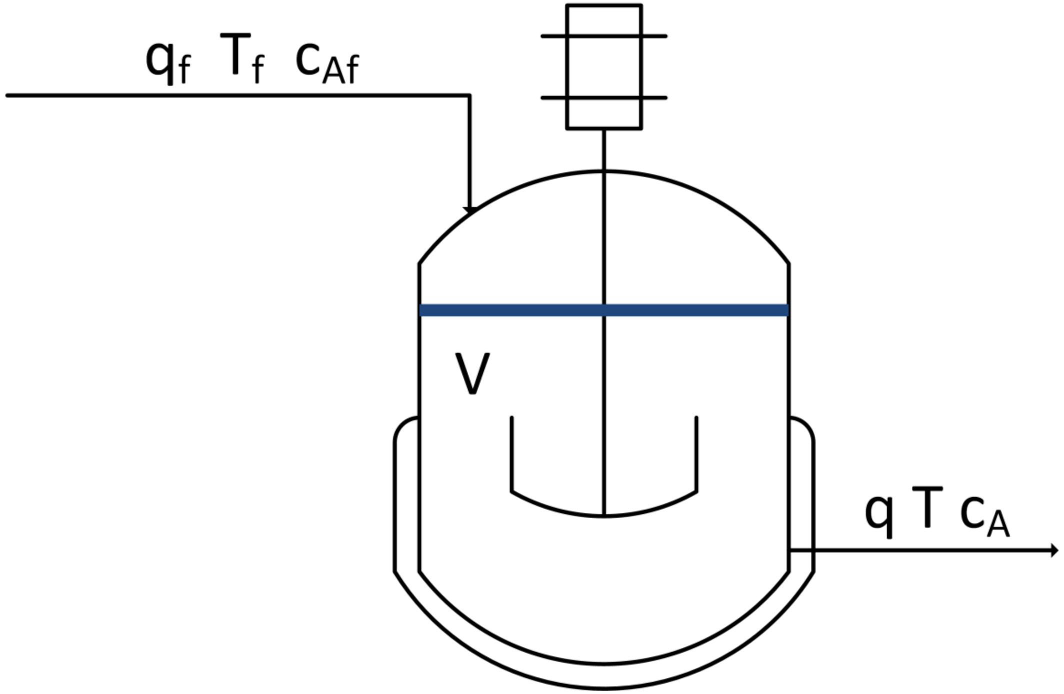
Apply chain rule

$$\frac{d(c_A V)}{dt} = c_A \frac{dV}{dt} + V \frac{dc_A}{dt}$$

$$c_A \frac{dV}{dt} + V \frac{dc_A}{dt} = c_{Af} q_f - c_A q$$

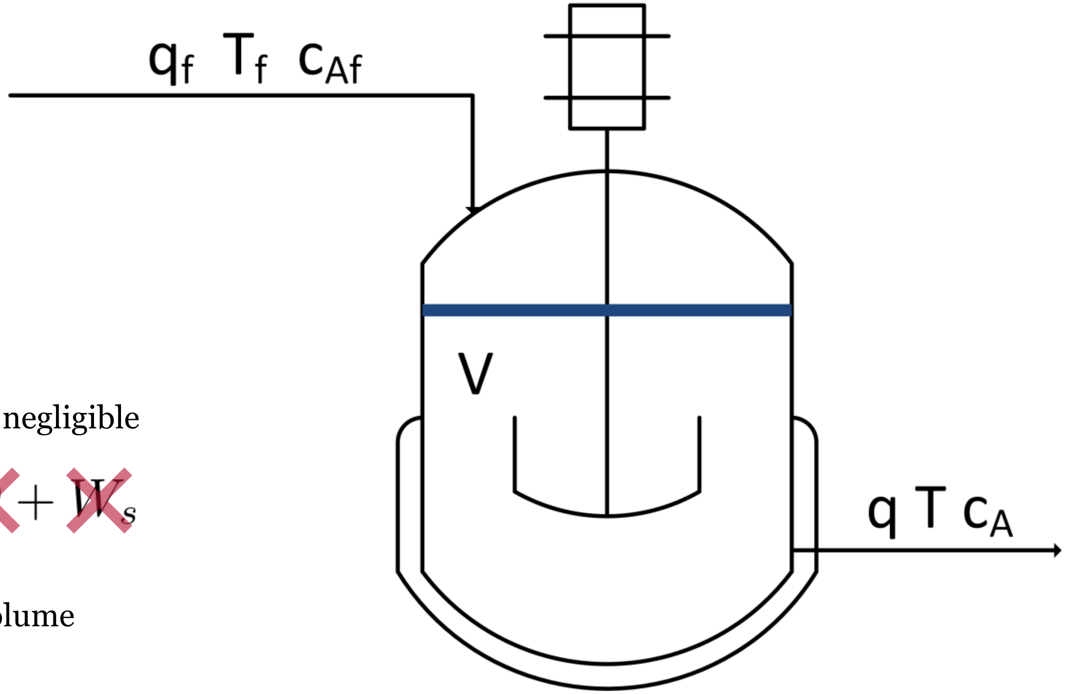
Rearrange terms

$$\frac{dc_A}{dt} = \frac{c_{Af} q_f - c_A q}{V} - \frac{c_A}{V} \frac{dV}{dt}$$



Note: We only use one species balance since this is a binary mixture and we already have an overall mass balance. Alternatively, we could have used two species balances and no overall mass balance.

CASE STUDY: DYNAMIC MIXER



5. Balances

- Energy balance

Let $T_{ref} = 0$, there is no heat added, and shaft work is negligible

$$c_p \frac{d(mT)}{dt} = \dot{m}_f c_p \left(T_f - \cancel{T_{ref}}\right) - \dot{m} c_p \left(T - \cancel{T_{ref}}\right) + \cancel{Q} + \cancel{W_s}$$

Divide out constant & equal heat capacity and introduce volume

$$\rho \frac{d(VT)}{dt} = \rho q_f T_f - \rho q T$$

Apply chain rule (also divide out the constant density)

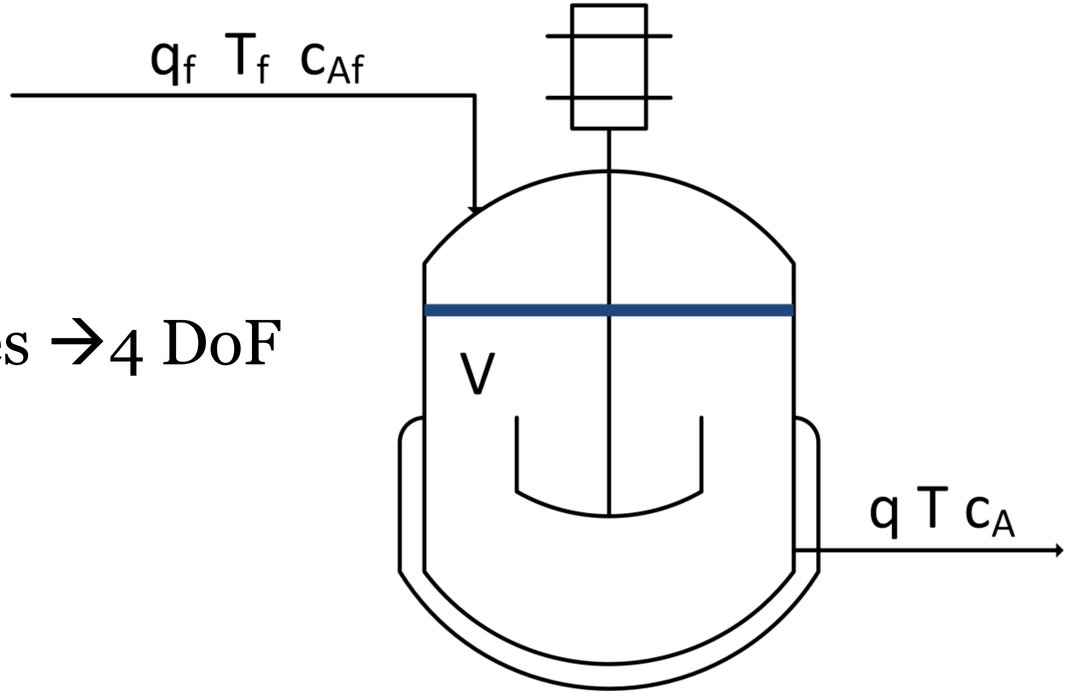
$$\frac{d(VT)}{dt} = T\frac{dV}{dt} + V\frac{dT}{dt}$$

$$T\frac{dV}{dt} + V\frac{dT}{dt} = q_f T_f - qT$$

Rearrange

$$\frac{dT}{dt} = \frac{q_f T_f - qT}{V} - \frac{T}{V}\frac{dV}{dt}$$

CASE STUDY: DYNAMIC MIXER



6. *Other relations:* None
7. *Degrees of freedom:* 3 equations, 7 variables →4 DoF
8. *Classify inputs:* q_f, T_f, C_{Af}, q (manipulated)
9. *Classify outputs:* V, T, c_A (states)
10. *Simplify balances:* already done!
11. *Steady-state:* inlets = outlets and V remains constant
12. *Dynamic response:* next time!

BEFORE WE MEET NEXT TIME

- Quiz 1: Due at 11:59pm tonight
- Read the syllabus
- Install Python on your computer using Anaconda
  - https://apmonitor.com/che263/index.php/Main/PythonIntroduction
- Prepare for the next lecture (~15 min.)
  - https://apmonitor.com/pdc/index.php/Main/SolveDifferentialEquations
- Start Assignment 1 (due Jan. 15)