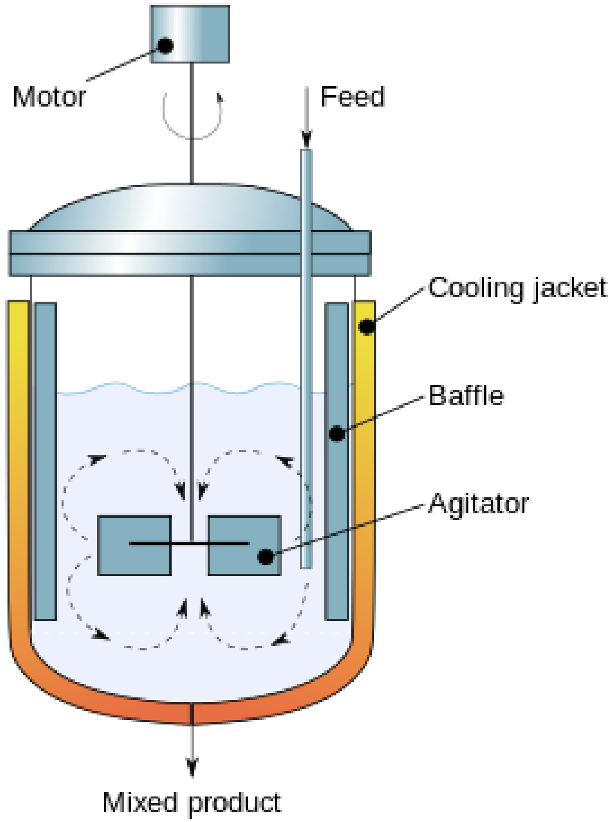
DYNAMIC BALANCES

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

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

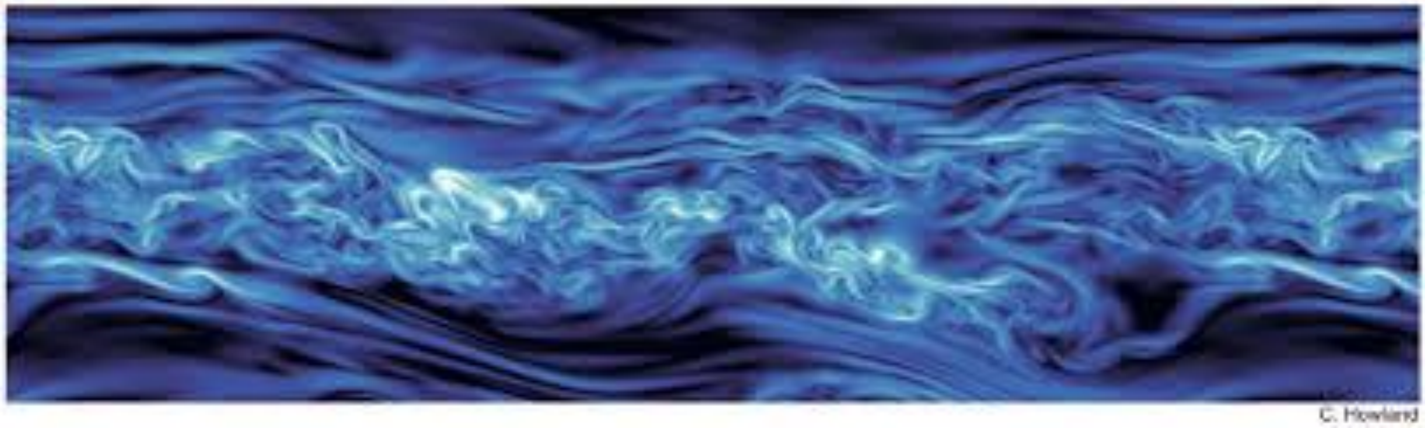
- Often reformulate in terms of concentration c_A and reaction rate r_A
  - Reaction rate is net molar generation per unit volume

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

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

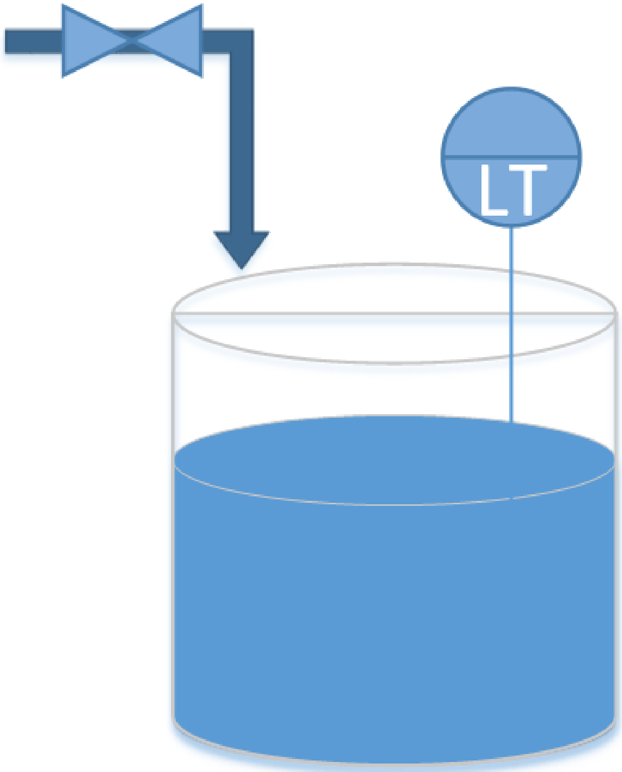
1. Identify objective for the simulation
2. Draw a schematic diagram, labeling process variables
3. List all assumptions
4. Determine spatial dependence
   - yes = Partial Differential Equation (PDE)
   - no = Ordinary Differential Equation (ODE)
5. Write dynamic balances (mass, species, energy)
6. Other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

DYNAMIC MODELING RECIPE (CONTINUED)

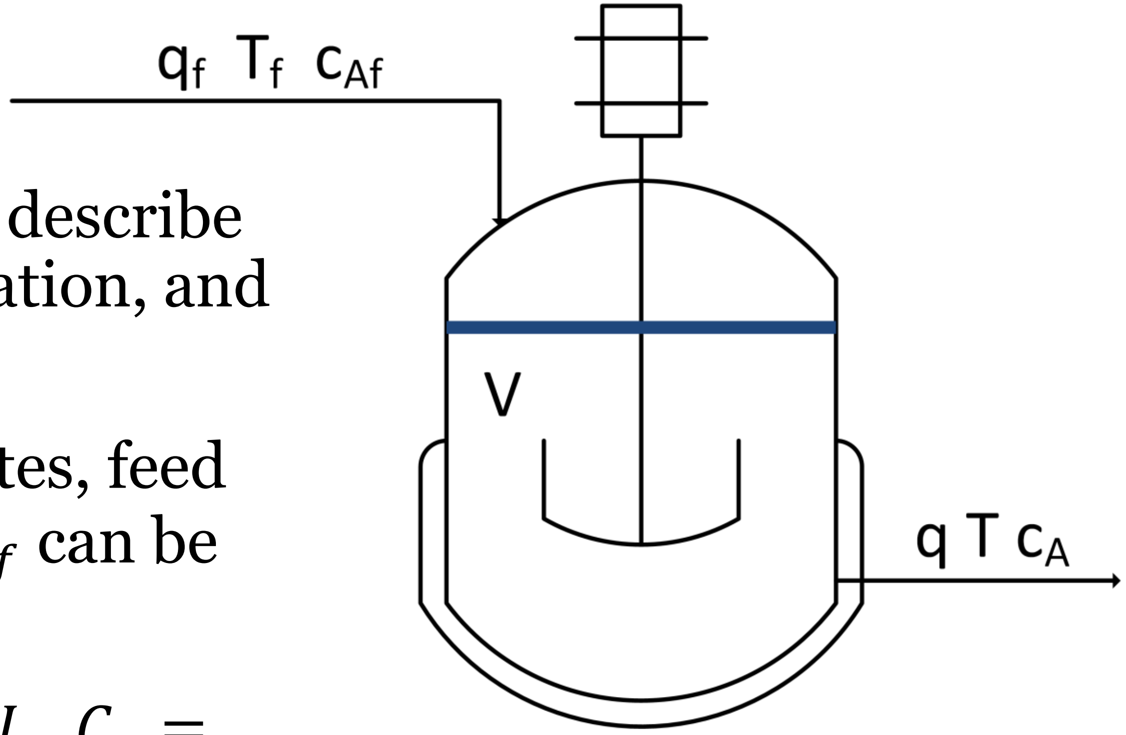
8. Classify inputs as
   - Fixed values
   - Disturbances
   - Manipulated variables
9. Classify outputs as
   - States
   - Controlled variables
10. Simplify balance equations based on assumptions
11. Simulate steady state conditions (if possible)
12. Simulate the output with an input step

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.



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.

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)