Lecture 3
Dynamic Modeling
Part II: Writing Balances for Lumped and Disritributed Parameter Systems

CHE4400

Professor Jay H. Lee
Georgia Inst. Technology

Lumped Parameter System

- Spatial dependence of variables is ignored.
  - Well-mixed system.
  - Systems with insignificant temperature or concentration gradient.
  - Variables are functions of time only, not spatial position.
  - Ordinary differential equation model.
- Examples
  - Mixer, CSTR
  - Tray of a distillation column
  - Steel ball for which heat conduction within is much faster than heat transfer to the surrounding.

Systematic Procedure

- Draw the control volume. Inside C.V., all intrinsic properties modeled should be assumed same.
- Identify which balances are needed.
  - Changing volume, height ⇒Total mass balance
  - Changing concentration ⇒Component molar or mass balance.
  - Changing temperature ⇒Energy balance
- Write down **mathematical expression for each term** appearing in the conservation equation – one by one.
- Put them together into equation.
- Use the chain rule, etc. to simplify.

Examples

- To become good at it, you must try many different problems. ⇒ Do the Extra Credit HW.
- Several additional examples are posted as notes.
  1. **Continuous Stirred Tank w/ Heater**
     - **Coupled mass and energy balance**
     - **Rate of heat release into the tank is chosen as independent variable (I.V.).**
  2. Electrically Heated Stirred Tank
     - Rate of energy addition to the heating coil is chosen as I.V.
     - Another energy balance is needed to model the dynamics of the coil temperature.
  3. Steam Heated Stirred Tank
     - Temperature difference between steam and heating coil is what drives the heat transfer.
     - “Quasi-steady-state” assumption for the coil temperature.

Examples

- In the notes….(continued)
  4. **Nonisothermal Batch Reactor**
     - **Component molar balances⇒concenrations**
     - **Energy balance ⇒temperature**
     - **Isothermal assumption – energy balance not needed.**
  5. Nonisothermal CSTR
     - Total mass balance ⇒height (volume)
     - Component molar balances⇒concentrations
     - Energy balance⇒temperature

Examples

- In the notes….(continued)
  6. Single component vaporizer
     - Liquid phase mass balance ⇒liquid volume
     - Vapor phase mass balance ⇒vapor-phase pressure
     - Liquid phase energy balance ⇒liquid temperature
     - Vapor phase energy balance ⇒vapor temperature
  7. Single component vaporizer (Simplified)
     - Assume thermal equilibrium: No vapor-phase energy balance.
     - Assume VL equilibrium ⇒vapor-pressure calculation (e.g., Antoine equation): No vapor-phase mass balance needed.

Examples

- In the notes….(continued)

8. Binary Distillation Column
   - Tray-by-tray (including condenser and reboiler) total mass and component mass balances
   - Assume vapor-liquid equilibrium (vapor phase mole fraction and liquid phase mole fraction are related).
   - Constant molar overflow (no energy balance needed).
   - Assume some liquid flow equation (Francis-Weir formula)
9. Staged Binary Absorber
   - Similar as distillation column if you assume trays are well-mixed for vapor-liquid equilibrium.

Distributed Parameter System

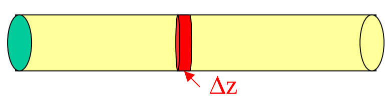
- Variables have spatial dependence
  - Instead of y(t), you have y(t,z) [1-dimeinsion] y(t,r,z) [2-dimeinsion] , or y(t,z,r,θ) [3-dimeinsion].
- Type of equation
  - Lumped parameter system ⇒ ODEs
  - Distributed parameter system ⇒ PDEs
- Example
  - Counter-current heat exchanger
  - Plug-flow reactor or packed-tube reactor
  - Heat conduction through a plate
  - Almost all systems show some spatial variations (e.g., due to imperfect mixing) but many systems can be treated as lumped parameter system.

Procedure for Obtaining PDEs

1. Determine the spatial dimension along which the variation is significant.
   - PFR- axial direction
   - Packed tube reactor with significant radial dispersion – axial and radial direction
   - Counter-current heat exchanger – axial direction
   - Heat conduction through a plate – x,y direction
   - Heat conduction through a sphere – radial direction
   - Continuous absorber – axial direction

Procedure for Obtaining PDEs

2. Choose a differential volume with respect to the selected spatial direction.



3. Develop a lumped parameter system model for the differential volume.
4. Draw spatial derivative terms by letting $\Delta z \to 0$.

$$\lim_{\Delta z \to 0} \frac{T(t, z+\Delta z) - T(t,z)}{\Delta z} = \frac{\partial T}{\partial z}(t)$$

5. Write down appropriate boundary conditions.

Examples in the Supplementary Notes

- **Double Pipe Steam Heat Exchanger**
  - **Axial variation on the tube side**
  - **Lumped parameter approximation in the shell side (steam side)**
- Plug Flow Reactor (Packed Tube Reactor)
  - Axial variation only
  - Ignore the radial dispersion $D_p \frac{\partial^2 C_A}{\partial r^2}(t)$

Solutions

- PDEs $\xrightarrow{\text{"Discretization"}}$ a large set of ODEs
- The large set of ODEs can be analyzed and simulated (integrated numerically) as before (using methods like Euler, RK, Gear).
- Discretization:
  - **Finite difference method**: After establishing a grid, use

$$\frac{\partial T}{\partial z} \text{ at } z = z_i \approx \frac{T(z_{i+1},t) - T(z_i,t)}{z_{i+1} - z_i} \text{ (forward difference)}$$

    to write down the equation for each grid point.
  - Finite element method

$$T(z,t) = \sum_{i=1}^{n} a_i(t)\phi_i(z),\ \ \phi_i(z): \text{polynomials of } z \Rightarrow \frac{\partial T}{\partial z} = \sum_{i=1}^{n} a_i(t)\frac{d\phi_i}{dz}$$

  - See the notes for details.