Mathematical Modeling

for Chemical Process Control

1. Types of mathematical models

a) First principles $$\frac{V}{F_{A,0}} = \int \frac{dX_A}{-r_A}$$

b) Empirical FOPDT, State Space, FIR, Neural Networks, etc.

c) Mixture of the two Semi-empirical

This lecture focuses on mathematical models based on first principles with either known or estimated parameters

2. Basic equations

- General conservation principle

$$\frac{\begin{bmatrix}\text{accumulation of } S\\ \text{within a system}\end{bmatrix}}{\text{time period}} = \frac{\begin{bmatrix}\text{flow of } S\\ \text{into the system}\end{bmatrix}}{\text{time period}} - \frac{\begin{bmatrix}\text{flow of } S\\ \text{out of the system}\end{bmatrix}}{\text{time period}} + \frac{\begin{bmatrix}\text{amount of } S\\ \text{generated within}\\ \text{the system}\end{bmatrix}}{\text{time period}} - \frac{\begin{bmatrix}\text{amount of } S\\ \text{consumed within}\\ \text{the system}\end{bmatrix}}{\text{time period}}$$

Accumulation = In - Out + Generation - Consumption

- where S can be:
  - total mass
  - mass of individual species
  - energy
  - momentum

3. Balances

- **Total Mass Balance:**

$$\frac{dm}{dt} = \frac{d(\rho V)}{dt} = \sum_{i=inlet} \dot{m}_i - \sum_{j=outlet} \dot{m}_j$$

$\dot{m}_i$ = mass flow rate of stream i

C_A = moles A / volume
q_i = volumetric flow rate of stream i

- **Species Mole Balance:**

$$\frac{dn_A}{dt} = \frac{d(c_A V)}{dt} = \sum_{i=inlet} c_{Ai} q_i - \sum_{j=outlet} c_{Aj} q_j + r_A V$$

- **Total Energy Balance:**

$$\frac{dE}{dt} = \frac{d(U+K+P)}{dt} = \sum_{i=inlet} w_i \left[h_i + \frac{z_i g_i}{g_c} + \frac{V_i^2}{2 g_c} \right] - \sum_{j=outlet} w_j \left[h_j + \frac{z_j g_j}{g_c} + \frac{V_j^2}{2 g_c} \right] + Q + W_s$$

h_i = enthalpy per unit mass of stream i

4. Forms of energy balance

- Neglecting potential and kinetic energy terms:

$$\frac{dE}{dt} = \frac{dU}{dt} = \sum_{i=inlet} w_i h_i - \sum_{j=outlet} w_j h_j + Q + W_s$$

- Note also that for liquid systems:

$$\frac{dU}{dt} \approx \frac{dH}{dt}$$

- In terms of temperature, the equation becomes (approximately):

$$\frac{d[\rho C_p V(T - T_{ref})]}{dt} = \sum_{i:inlet} w_i C_p (T_i - T_{ref}) - \sum_{j:outlet} w_j C_p (T_j - T_{ref}) + Q + W_s$$

- We will <u>not</u> be using a momentum equation in this class.

How to Develop a Transient Model (Table 2.1)

1. Identify objective
2. Draw a schematic diagram, labeling process variables
3. List all assumptions
4. Determine spatial dependence
    - yes = PDE
    - no = ODE
5. Write dynamic balances (mass, species, energy)
6. Other relations (thermo, reactions, geometry, etc.)
7. Degrees of freedom
    - Does # of eqns = # of unknowns?
8. Simplify (outputs on LHS, inputs on RHS)
9. Classify inputs as
    - Disturbances
    - Manipulated variables