# Mathematical Modeling

ChE 436

Class 13

### 1. Types of mathematical models

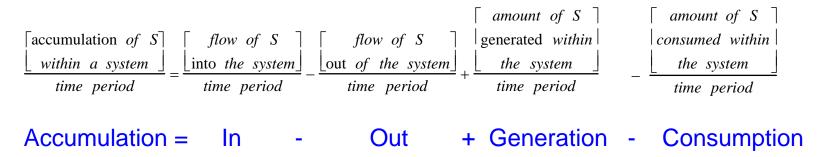
a) First principles  $\frac{V}{F_{A,0}} = \int \frac{dX_A}{-r_A}$ 

- b) Empirical FOPDT for everything
- c) Mixture of the two Semi-empirical

We will focus on mathematical models based on first principles in this chapter (Chapter 2)

## 2. Basic equations

General conservation principle



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

#### 3. Balances

Total Mass Balance:

$$\frac{dm}{dt} = \frac{d(\rho V)}{dt} = \sum_{i=inlet} w_i - \sum_{j=outlet} w_j$$

w<sub>i</sub> = mass flow rate of stream i

Species Mole Balance:

C<sub>A</sub> = moles A / volume q<sub>i</sub> = volumetric flow rate of stream i

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

Total Energy Balance:

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

h<sub>i</sub> = 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 <u>momentum</u> equation in this class.

 What assumption does this book make about heat capacities?

# 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