

Mathematical Modeling Examples

ChE 436
Class 15

How to Develop a Transient Model (simplified)

1. Draw a schematic diagram, labeling process variables
2. List all assumptions
3. Make sure it is an ODE (no spatial dependence)
4. Write dynamic balances (mass, species, energy)
5. Other relations (thermo, reactions, geometry, etc.)
6. Degrees of freedom
 - Does # of eqns = # of unknowns?
7. Simplify

Balances

- **Total Mass Balance:**

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

- **Species Mole Balance:**

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

- **Total Energy Balance:**

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