Chemical Engineering 436
Mathematical Modeling

1. Types of mathematical models

a. First principles
b. Empirical
c. Mixture of the two

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

2. Basic equations

General conservation principle

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

where S can be: Total mass, mass of individual species, energy, momentum

Total Mass Balance:

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

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:

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

or, 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.

What assumption does this book make about heat capacities?