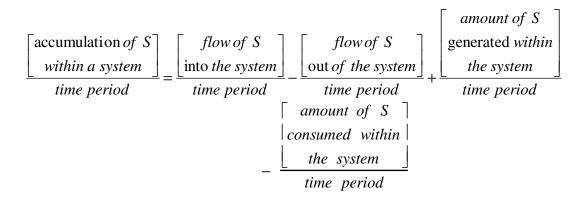
## 1. Types of mathematical models

- 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



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?