ABE 201
Biological Thermodynamics 1

Module 13: Integrated Mass and Energy Balances (1st and 2nd Law)

Outline

- Review of mass and energy balance equations

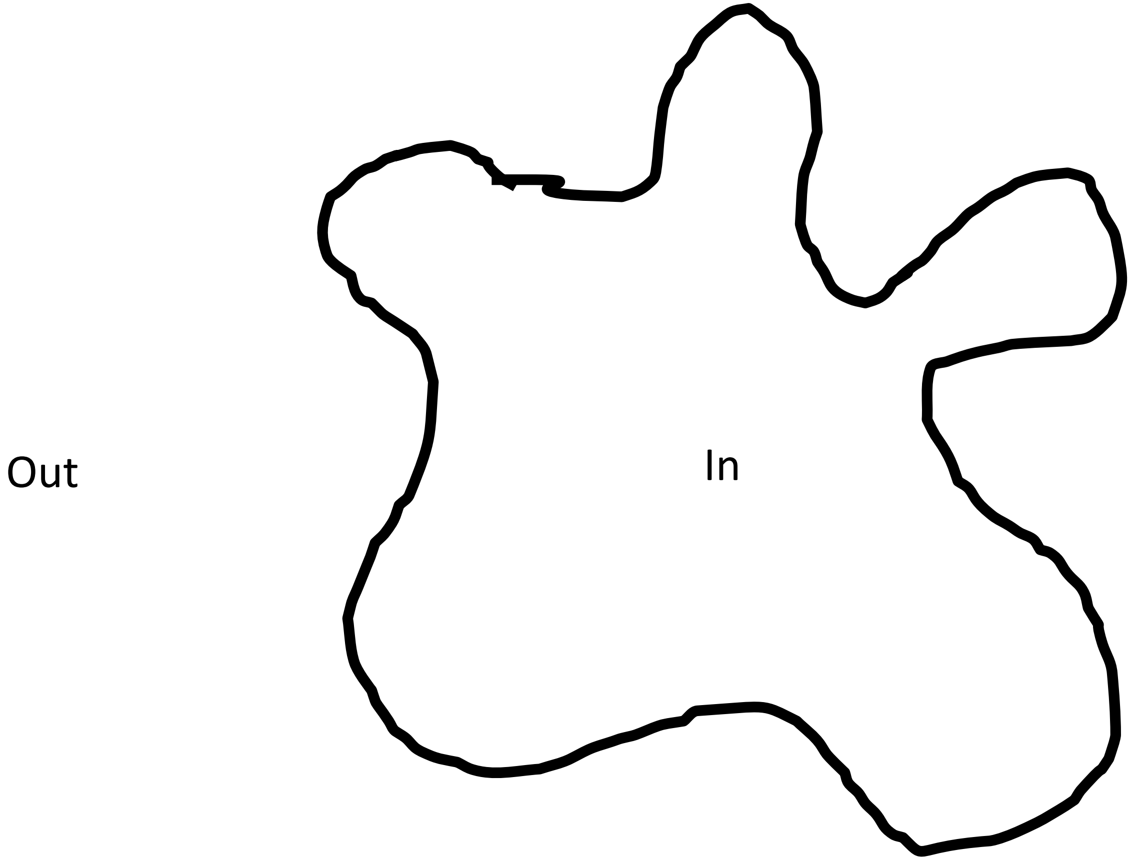
- Strategies for solving mass and energy balances

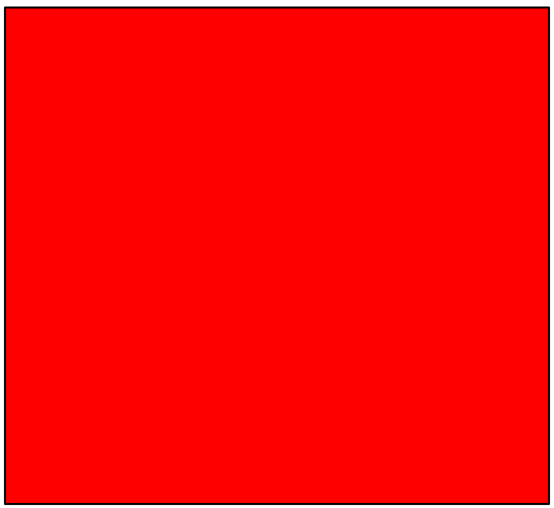
Generalized Continuity Equation

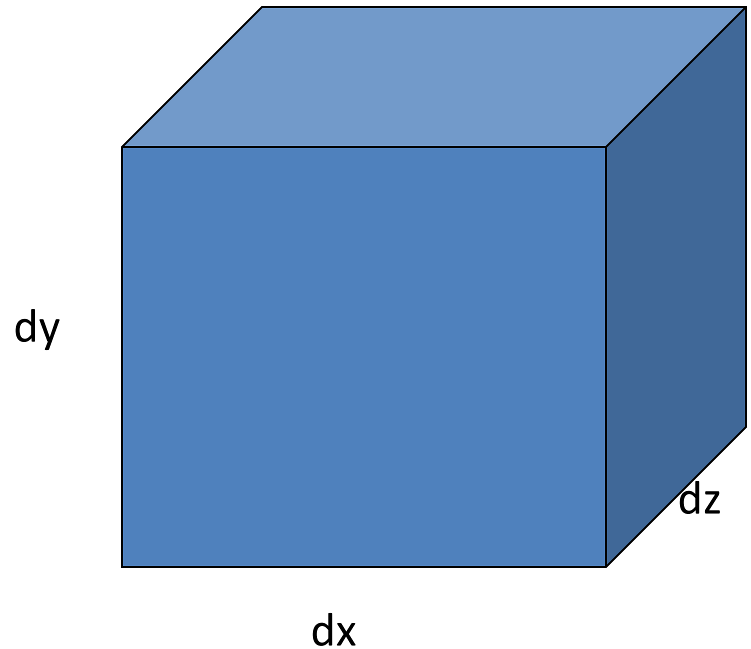
Accumulation = in – out + generation - consumption

- Mass balances
- Energy balances (1st and 2nd law)
- Non-steady state thermodynamics
  - Maxwell's equations
- Momentum balances
  - Fluid mechanics
  - Navier Stokes equation
- Heat/mass transfer
  - Fickian diffusion
- Chemical kinetics
  - 1st order, 2nd order reactions
  - Michaelis-Menten enzyme kinetics
- Cellular growth models

System Definition






dy
dz
dx

Conservation of Mass

Accumulation = In – Out + Generation - Consumption

- **Steady-state: Accumulation = 0**

- **No chemical Reactions: Gen = Con = 0**

- **Chemical Reactions?**
  - **Two Approaches**
  - **Atomic Species Balance**
  - **Chemical Compound Balance**

$$dX_i = \sum_{in} \dot{m}_{in} \cdot x_{i,in} dt - \sum_{out} \dot{m}_{out} \cdot x_{i,\mathrm{out}} dt + \sum \nu_i \cdot \xi \cdot MW_i \cdot dt$$

$$\frac{dX_i}{dt} = \sum_{in} \dot{m}_{in} \cdot x_{i,in} - \sum_{out} \dot{m}_{out} \cdot x_{i,\mathrm{out}} + \sum \nu_i \cdot \xi \cdot MW_i$$

1st Law Energy Balances

Accumulation = In – Out + Generation - Consumption

Closed System Energy Balance

$$\Delta U + \Delta E_k + \Delta E_p = Q - W$$

Open System Energy Balance

$$\Delta \dot{H} + \Delta \dot{E}_k + \Delta \dot{E}_p = \dot{Q} - \dot{W}_s$$

Open System Energy Balance

$$\cancel{\frac{d\dot{H}}{dt}}+\cancel{\frac{d\dot{E}_k}{dt}}+\cancel{\frac{d\dot{E}_p}{dt}}=\left(\dot{Q}_{in}-\dot{Q}_{out}\right)-\left(\dot{W}_{s,out}-\dot{W}_{s,\mathrm{in}}\right)$$

$$+\left(\dot{H}_{in}-\dot{H}_{out}\right)$$

$$+\left(\dot{E}_{k,in}-\dot{E}_{k,out}\right)$$

$$+\left(\dot{E}_{\mathrm{P},in}-\dot{E}_{\mathrm{P},out}\right)$$

Steady State
Open System Energy Balance

$$0 = \dot{Q} - \dot{W}_s +$$

$$\sum \dot{m}_{in} \cdot \hat{H}_{in} - \sum \dot{m}_{out} \cdot \hat{H}_{out} +$$

$$\sum \tfrac{1}{2} \dot{m}_{in} \cdot v_{in}^2 - \sum \tfrac{1}{2} \dot{m}_{out} \cdot v_{out}^2 +$$

$$\sum \dot{m}_{in} \cdot g \cdot z - \sum \dot{m}_{out} \cdot g \cdot z$$

Rearranging:

$$\sum \dot{m}_{out} \cdot \hat{H}_{out} - \sum \dot{m}_{in} \cdot \hat{H}_{in} +$$

$$\sum \tfrac{1}{2} \dot{m}_{out} \cdot v_{out}^{2} - \sum \tfrac{1}{2} \dot{m}_{in} \cdot v_{in}^{2} +$$

$$\sum \dot{m}_{out} \cdot g \cdot z - \sum \dot{m}_{in} \cdot g \cdot z =$$

$$\dot{Q} - \dot{W}_{s}$$

Finding Enthalpy Changes

$$\Delta\dot{H} = \dot{H}_{out} - \dot{H}_{\mathrm{in}}$$

$$\Delta\dot{H} = \left[\Sigma\left(\hat{H}_{i,out}\dot{m}_{i,out}\right) - \Sigma\left(\hat{H}_{i,\mathrm{in}}\dot{m}_{i,\mathrm{in}}\right)\right]$$

$$\Delta\dot{H} = \Delta\hat{H}_{sensible}\dot{m} + \Delta\hat{H}_{latent}\dot{m}$$

$$\Delta\dot{H} = \int_{T_1}^{T_2} C_p dT \cdot \dot{m} + \Delta\hat{H}_{latent}\dot{m}$$

$$\Delta\dot{H} = \int_{T_1}^{T_2}\left(a + bT + cT^2 + dT^3\right)dT \cdot \dot{m} + \Delta\hat{H}_{latent}\dot{m}$$

2nd Law Balances

Accumulation = In – Out + Generation - Consumption

$$\Delta S_{sys} = S_{in} - S_{out} + S_{gen}$$

$$\frac{dS_{sys}}{dt} = \dot{S}_{in} - \dot{S}_{out} + \dot{S}_{gen} \quad \text{(rate form)}$$

$$S_{gen} \geq 0$$

Finding S_{in} and S_{out}

1. Entropy transfer associated with heat transfer

$$S_{heat} = \frac{Q}{T} \quad \text{(T=constant)} \quad \text{for adiabatic, } S_{heat} = 0$$

$$S_{heat} = \int_1^2 \frac{\delta Q}{T} \quad \text{(when T is not constant)}$$

2. Entropy transfer associated with mass flow

$$\dot{S}_{mass} = \dot{m}\hat{s}$$

$$\dot{S}_{mass} = \dot{m}\hat{s} = 0 \quad \text{(for no mass flow, closed system)}$$

2^{nd} Law Balances

Closed Systems (m = 0)

$$dS_{sys} = \int \frac{dQ_k}{T_k} dT + S_{gen}$$

Open Systems (m > 0)

$$\cancel{dS_{sys}} = \sum \frac{Q_k}{T_k} + \sum m_{in}\hat{s} - \sum m_{out}\hat{s} + S_{gen}$$

Steady state/flow

Adiabatic Systems (Q =0)

$$\cancel{dS_{sys}} = \sum m_{in}\hat{s} - \sum m_{out}\hat{s} + S_{gen}$$

Solving Combined Mass and Energy Balances

1. Make a diagram!
2. Organize the information given on diagram and/or figure.
3. Identify the unknowns.
4. Write mass balance equation(s). Solve if possible
5. Write 1st law energy balance equation. Solve if possible
6. Write 2nd law energy balance equation. Solve if possible.
7. Combine mass and energy balances to solve

Summary

- The generalize continuity equation can be used to derive mass and energy (both 1st and second law) balance equations.
- Enthalpy values can be obtained by calculation or from tabulated values
- Entropy values can be obtained from tabulated values (or calculated – but not until next semester!)
- Solving complex problems may require simultaneous solving of your mass and energy balance equations