Chapter 3 – Conservation of Mass and Chemical Species Accounting

1. Define, illustrate, compare and contrast the following terms and concepts:

Mass
- mass vs. weight
- units of measurement
  - mass: m (kg, g, lbm, slug)
  - amount of substance: n (kmol, gmol, lbmol, slugmol)
    - (most useful when chemical reactions are involved)
- molecular weight (molecular mass): M (kg/kmol, g/gmol, lbm/lbmol)
  - relationship between m and n
  - density & specific volume (how are they related?)
  - specific weight vs. specific gravity (how are they different?)

Application of Accounting Principle for Mass
- rate of accumulation of mass within the system

amount of mass within the system: $\boxed{m_{sys} = \iiint_V \rho \, dV}$

- density vs. specific volume (ρ vs v)
- transport rate of mass across system boundaries
  - mass flow rate: $\boxed{\dot{m} = \iint_{A_c} \rho \, V_n \, dA}$ (kg/s, lbm/s)
  - volumetric flow rate: $\dot{V} = \iint_{A_c} V_n \, dA$ (m³/s, ft³/s)
    - where A_c = cross-sectional area
  - molar flow rate : $\dot{n} = \dot{m}/M$ (kmol/s, mol/s,lbmol/s):
  - local normal velocity: V_n
  - one-dimensional flow assumption
  - average velocity at a cross-section: V_{AVG}
    - mass and volumetric flow rate based on average velocity:

$$\boxed{\dot{m} = \rho \, A_c V_{AVG}} \quad \& \quad \boxed{\dot{V} = A_c \, V_{AVG}}$$

- generation/consumption rate of mass within the system
  - Empirical result ----- Mass is conserved! It's really a conservation principle!

conservation of mass equation

rate form $$\frac{dm_{sys}}{dt} = \sum \dot{m}_{in} - \sum \dot{m}_{out}$$

finite-time form $$m_{sys,\,final} - m_{sys,initial} = \sum m_{in} - \sum m_{out}$$

Chemical Species (Compounds)

units of measurement --- same as for mass

m_i = mass of component i

n_i = moles of component i $\quad n_i = m_i / M_i$

mixture composition

moles of mixture: $\boxed{n = \sum_{i=1}^{N} n_i}$

where N = number of components in the mixture

mole fractions: $nf_i = \frac{n_i}{n_{mix}}$ and $\boxed{\sum_{i=1}^{N} nf_i = 1}$

mass of mixture: $\boxed{m = \sum_{i=1}^{N} m_i}$

mass (weight) fractions: $mf_i = \frac{m_i}{m_{mix}}$ and $\boxed{\sum_{i=1}^{N} mf_i = 1}$

Application of Accounting Principle for Chemical Species

rate of accumulation of component i within the system

amount of component i within the system:

$\boxed{m_{i,sys} = \iiint_V \rho_i \, dV}$ and $\boxed{n_{i,sys} = \frac{m_{i,sys}}{M_i}}$

transport rate of component i across system boundaries

mass flow rate of component i : $\dot{m}_i$ (kg/s, lbm/s, slug/s)

molar flow rate of component i : $\dot{n}_i$ (kmol/s, mol/s, lbmol/s)

generation/consumption rate of species i within the system

chemical reactions and generation/consumption

balanced reaction equations and consumption/generation terms

generation (production or creation) rate: $\dot{m}_{i,gen}$ or $\dot{n}_{i,gen}$

consumption (destruction) rate: $\dot{m}_{i,con}$ or $\dot{n}_{i,con}$

chemical species accounting equation (mass basis)

rate form $$\frac{dm_{i,sys}}{dt} = \sum \dot{m}_{i,in} - \sum \dot{m}_{i,out} + \dot{m}_{i,gen} - \dot{m}_{i,con}$$

finite-time form $$m_{i,sys,final} - m_{i,sys,initial} = \sum_{in} m_{i,i} - \sum_{out} m_{i,e} + m_{i,gen} - m_{i,con}$$

chemical species accounting equation (mole basis)

rate form

$$\frac{dn_{i,sys}}{dt} = \sum \dot{n}_{i,in} - \sum \dot{n}_{i,out} + \dot{n}_{i,gen} - \dot{n}_{i,con}$$

finite-time form

$$n_{i,sys,final} - n_{i,sys,initial} = \sum n_{i,in} - \sum n_{i,out} + n_{i,gen} - n_{i,con}$$

Constitutive relation
Examples: Ohm's Law, Ideal Gas Model

Ideal Gas Model
universal gas constant R_u vs. specific gas constant R

2. Given one of the species accounting or conservation of mass equations and a list of assumptions, carefully indicate the consequences of each assumption. Typical assumptions include: steady-state, one-inlet/one-outlet, closed system, open system, and no chemical reactions.

3. Given one of the species accounting or conservation of mass equations, explain what each term represents physically and how it relates to the overall accounting framework discussed in Chapters 1 and 2.

4. Given information about the local velocity distribution and density distribution at the boundary of a system, calculate the mass flow rate and the volumetric flow rate at the boundary.

5. Given a mixture composition in terms of either mass (weight) fractions or mole fractions, determine the composition in the other measure. If total mass of the mixture is specified, determine the moles or kilograms of each component in the mixture. (Best done using a simple table format.)

6. Given a problem that can be solved using conservation of mass and species accounting, you should be able to do the following tasks:
   (1) Select an appropriate system. Identify the system and its boundaries on an appropriate drawing. Describe the system and its boundaries in sufficient detail so that there is no confusion about your choice. Indicate whether the system is open or closed.
   (2) Indicate the time interval appropriate for the problem (e.g. should you use the rate-form or the finite-time form?).
   (3) Clearly identify and count the number of unknowns you are trying to find. Define and use a unique symbol for each unknown.
   (4) Develop a set of INDEPENDENT equations that are equal in number to the number of unknowns and are sufficient to solve for the unknowns. These equations are developed using conservation of mass, species accounting, and information given in the problem statement, e.g. physical constraints and constitutive equations.
   (5) Solve for the unknown quantities.
   (6) Substitute in the numerical values to find a numerical answer.

7. Given a problem with non-uniform chemical composition, i.e. a separation, distillation or a mixing problem, apply conservation of mass and species accounting to solve for the unknown mass flow rates or masses and mixture compositions.

8. Given a numerical value for one of the following quantities determine the numerical value of the remaining quantities:

   density, specific volume, specific weight, specific gravity

9. Given any two of the following properties—pressure, temperature, and density (mass or molar)—use the ideal gas equation to find the unknown property.