Chapter 2 Introduction to Engineering Calculations

(Refs: Geankoplis CJ: Sec. 1.1 to 1.4. and Exercises: 1.2-1 to 1.4-3. Felder RM & Rousseau RW: Chapters 1-3. Himmelblau DM: Chapter 1)

Process technology involves physical or chemical changes of materials. Quantification of the process variables and conditions, and the amounts of materials and energy is essential for the design, operation, analysis (or diagnosis), productivity and economy of the process. Therefore, mathematics is both a language and a tool of engineering and process technology. Nevertheless, the calculations involved in this subject only require simple and basic math. The difficulties for most students in learning this subject are more in the understanding the physical concepts of processes but not to using mathematical equations. This subject is to use mathematics to solve process technology problems but not to study pure math.

Example 1 For the evaporation process shown in Fig. 1, given the flow rate F, solute concentration X_F and temperature T_F of the feed solution, and the desired concentration of the concentrated solution x_L , we can ask several quantitative questions.

- (1) The amount of vapor *V* generated?
- (2) The amount of concentrated solution *L*?
- (3) The amount of steam *S* required?
- (4) The heat transfer area required?
- (5) The volume of evaporator?

Fig. 1 Evaporation process, heat and mass balances (*x*-conc, *H*-enthalpy, *B*-boiling pt.)

This chapter is to introduce the basic terms and major process variables which are encountered in this subject. **It is imperative that you understand and be very familiar with** these terms and their physical meanings. Memorise as many of these terms as you can and do a lot of exercises.

1. Dimension and Units

- A **dimension** is a property that can be measured, such as length (*L*), mass (*M*), time (*θ*) and temperature (*T*).
- A **unit** is a quantitative measurement of the dimension, such as meters (m) for length, kilograms (kg) for mass, seconds (s) for time and degrees Celsius ($\rm{^o}C$) for temperature.

To quantify a property, you need **both a numerical value and a unit**, e.g., the pressure of a gas in a container is 50 kPa. (Neither the value 50 nor the unit kilopascal by itself can define the level of pressure). In many cases, the unit of a property can tell you the definition.

1.1. Dimensional consistency

Dimensional consistency is a general rule for the use of mathematical equations to express physical relationships. It requires that, in an equation of physical relationship, all the *additive* terms on both sides of the equation must have the same net dimension. For example, the van de Waals equation,

 $(p + a/V^2) (V-b) = RT$

To satisfy the rule of dimensional consistency, (1) the term a/V^2 must have the dimension of pressure, so that the constant *a* has the dimension of (pV^2) , and (2) the constant *b* should bear volume dimension.

A straightforward interpretation of the dimensional consistency rule is that you can only add or subtract physical terms of the same dimension. Apparently, $1 \text{ kg (mass)} + 2 \text{ m (length)} -$ 0.5 L (volume) makes no sense. You may divide or multiply, but may not add or subtract different properties and units (because they are not the same thing).

Examples:

(1) A sugar solution has a conc of 0.03 kg/L, so that 5 m^3 of the solution contains

 5 m^3 x 0.3 kg/L = 5000 L (0.03 kg/L) = 150 kg sugar

(2) A car with a weight 1000 kg traveling on the road at a speed of 60 km/h has a kinetic energy of $E_K = \frac{1}{2}mv^2 = \frac{1}{2}(1000 \text{ kg})(60,000 \text{ m}/3600 \text{ s})^2 = 1.389 \times 10^5 \text{ kg} - \frac{\text{m}^2}{\text{s}^2} = 1.389 \times 10^5$ J.

(3) However: 150 kg sugar + 5 m³ water =? or 1000 kg + 60 km/h = ?

Dimensionless groups are formed by putting groups of variables together with all their units cancelled out. For example, the **Reynolds number**, defined (for fluid flowing in pipe) as,

Re= Duρ/μ

is a very useful dimensionless group in fluid mechanics, and heat and mass transfer processes $(D =$ pipe diameter *L*, $u =$ velocity L/θ , $\rho =$ density M/L^3 and $\mu =$ viscosity of fluid M/L - θ). In process technology and chemical engineering many design equations are correlations of dimensionless groups.

1.2. Unit systems

A property can be expressed with different units, e.g., mass: kilogram, gram, pound; length: meter, millimetre, feet. The use of various unit systems is a matter of convention and convenience. Various unit systems may be classified into two main groups: *Metric System* and *English System*:

- **Metric Units:** including CGS (cm-g-s system), SI (International System)
- **English Units:** including FPS (ft-lb-s or English absolute), and

Gravitational Systems: British Engineering, American Engineering

(Ref: http://www.onlineconversion.com/)

The SI system is most commonly used in the scientific community, and the American Engineering system of units is dominant in the United States. In this subject, SI units are used in most cases, and English units used in fewer cases. You must be familiar with these units and their conversion. The basic units in these unit systems are summarised in **Table 1**.

Important: When calculating an unknown variable (*y*) from other known variables $(x_1, x_2,$ x_3, \ldots) with an equation $(y = f(x_1, x_2, x_3, \ldots))$, you should substitute **both the values and the units** of the known variables into the equation. Then, both the value and unit for the unknown variable should be *derived* (*calculated*) from the equation. To guard against errors during the calculation, it is wise for you to convert all the variables into one unit system before substituting them into the equation.

Note: (1) The hyphen "-" between two units means times or multiplication, and it is sometimes replaced by a central dot " \bullet " or a space.

(2) K and ${}^{\circ}R$ are all absolute temperature scales while ${}^{\circ}C$ and ${}^{\circ}F$ are relative scales.

(3) " \equiv " means "always equal" or "is defined as".

(4) Length, time, mass and temperature are *base* dimensions for deriving all other dimensions in the table.

2. Common physical properties of material and process technology terms

- **- Density (** ρ **)**: the mass per unit volume (kg/m³, g/cm³, lb_m/ft³)
- **- Specific Volume (***v***): the volume per unit mass** $(m^3/kg, cm^3/g, ft^3/lb_m)$ **,** $\rho=1/v$
- **Specific Gravity (SpGr)**: the ratio of density to the density of a reference. Unless otherwise specified, the reference substance for solids and liquids is normally water at 4° C (ρ =1000 kg/m³ =1.0 g/cm³ = 62,43 lb/ft³); the reference for gases is air. Since the density of water is equal to 1.0 $g/cm³$, and the specific gravity of solid and liquid is numerically equal to its density (in g/cm^3).
- **Viscosity (μ)**: a measure of the property of a fluid resisting flow and deformation. The most common unit of viscosity is *centipoise*(cp),

1 cp=0.01 p (poise=g/cm-s)=10⁻³ Pa-s (kg/m-s)=6.7197×10⁻⁴ lb_m/ft-s

Most physical properties of materials are dependant on temperature, pressure and state (solid, liquid and gas). Therefore, these conditions must be specified when using the value of a physical property.

3. Process variables

3.1. Temperature

The temperature of an object is a measure of its thermal state considered in reference to its power to transfer heat to other body. Temperature is normally measured in degrees Celsius ^oC and Fahrenheit^oF, which are defined on different bases. The Celsius scale is based on the physical state of water, i.e., 0° C corresponds to the freezing point of water, and 100° C to the boiling point (**Table 2** and diagram).

Both Celsius and Fahrenheit scales are *relative* scales, with arbitrarily fixed zero points. *Absolute* temperature scales have their zero points set at the lowest temperature that can exist. The absolute scale corresponding to Celsius is called the **Kelvin** scale (K), its zero point is - 273.15^oC; and corresponding to the Fahrenheit is the **Rankine** scale (^oR), and 0^oR is equal to -459.67 °F. The relationships between these temperature scales and temperature differences/changes,

> $K = {}^{o}C + 273.15,$ ${}^{o}R = {}^{o}F + 459.7$ ${}^{o}F = 1.8(^{o}C) + 32,$ ${}^{o}R = 1.8(K)$ $\Delta(^{\circ}C) = \Delta(K), \ \Delta(^{\circ}F) = \Delta(^{\circ}R)$

Fig. 2 Various temperature scales and relationship.

To further illustrate these temperature conversion equations, you may apply them to the temperatures in the following table and chart. For example, the water boiling $T = 100 \degree C$,

- 1) $K = {}^{0}C + 273 = (100 + 273), T = 373 K$
- 2) ${}^{0}F = 1.8({}^{0}C) + 32 = 1.8x(100) + 32 = 212$, T= 212 ${}^{0}F$
- 3) ${}^{0}R = ({}^{0}F) + 460 = 212 + 460 = 672$, T =672 ${}^{0}R$
- 4) or ${}^{\circ}R = 1.8(K) = 1.8(373) = 672$, T = ${}^{\circ}R$

The conversion from 1-3 is to find out the *equivalent* temperature in another scale.

Note: The ^oC and ^oF in the units of some physical properties actually mean **Δ**^oC and **Δ**^oF, such as those in heat capacity C_p (kJ/kg- $\rm{^o}C$, Btu/lb- $\rm{^o}F$).

Test yourself questions:

Q1: Show that temperature, ${}^{\circ}R = 1.8$ (K), such as 298 K = 1.8(298) ${}^{\circ}R = 536.4{}^{\circ}R$

Q2: Convert heat capacity C_p in kJ/kg^{-o}C to Btu/lb-^oF, given 1 btu = 1.055 kJ, 1 kg = 2.2 lb and above equations. Which one of the following is right?

1) 1 kJ/kg^{-°}C=
$$
\frac{1 \, btu}{1.055} \frac{1}{2.2 \, lb} \frac{1}{(1.8 \times 1 + 32)^\circ C} = \frac{0.431 \, btu/lb}{33.8^\circ F} = 0.01275 \, btu/lb
$$
-°C
2) 1 kJ/kg^{-°}C = $\frac{1 \, btu}{1.055} \frac{1}{2.2 \, lb} \frac{1}{1.8^\circ F} = \frac{0.431 \, btu/lb}{1.8^\circ F} = 0.2394 \, btu/lb$ -°F

Q3: $1 \text{ }^{\circ}C = ? \text{ }^{\circ}F = ? K = ? \text{ }^{\circ}R$. Which one of the following is right?

Answer 1: $1^{\circ}C = 1.8^{\circ}F = 1$ K = $1.8^{\circ}R$

Answer 2: $1 \text{ }^{\circ}C = 1.8 \text{ } (1) +32 = 33.8 \text{ }^{\circ}F = 273 + 1 = 274 \text{ K} = 33.8 + 460 = 493.8 \text{ }^{\circ}R$

Q4: Because 25 °C = 25 + 273 K = 298 K = 1.8 (25) +32 = 77 °F, 1 °C = 298/25 = 11.92 K or $77/25 = 3.08$ °F. Correct or not, and why?

(You can only say *each* $\rm{^oC}$ is equal to *how many* K or *how many* $\rm{^oF}$ for a temperature interval or change but not for the specific temperature level.)

3.2. Pressure

The pressure on an object is defined as the *normal* force per unit surface area of the object (pressure = force/area). The pressure in process technology is mostly related to fluid pressure, i.e., the pressure of a gas or liquid in a container, a process unit or during fluid transportation. The following pressure terms or scales are often used, absolute pressure gauge pressure p_g and vacuum p_{vac} (Fig.3).

1) Atmospheric pressure p_{atm} , is the pressure due to the weight of the gaseous layer or the atmosphere surrounding our planet. Since atmospheric pressure is measured with a barometer, it is also called the **barometric pressure**.

2) Gauge pressure (*pg*): the pressure *relative to* or *over* the atmospheric pressure.

3) Absolute pressure (*pabs*): the pressure *relative to* absolute or *perfect vacuum*. Obviously,

$$
p_{\scriptscriptstyle abs} = p_{\scriptscriptstyle atm} + p_{\scriptscriptstyle g}
$$

4) Vacuum is a measure of pressure level *below* the atmospheric pressure, *Vac = patm− pabs* (where *pabs* < *patm*). Therefore, zero vacuum means that the pressure equals the atmospheric pressure, and 5 in.Hg vacuum means that the pressure is 5 in.Hg below the atmospheric pressure, or the absolute pressure is (*patm−*5 in.Hg).

Standard pressure is corresponding to 1 atm = 760 mm Hg (at 0° C). However, the atmospheric pressure p_{atm} at a given location is not always 1 atm (mostly not).

Fig. 3 Various pressure scales and relationship.

Manometer is a simple type of pressure meter for fluid at low pressures (below 3 atm). The most common form of manometer consists of a glass U-tube filled with a liquid of known

density $(\rho_f$ for the manometer liquid, Fig. 4). When the two ends of the U-tube are exposed to different pressures p_1 on the left and p_2 on the right, the liquid level drops in the high pressure arm and rises in the low pressure arm, and the pressure difference is given by

$$
p_1 - p_2 = (\rho_f - \rho)gh
$$

where ρ is the density of fluid being measured. If the fluid is a gas, ρ ^{*<*}*<* ρ *_f*, ρ _f^{\rightarrow} ρ ^{\approx} ρ _{*f*}, and p ₁ \rightarrow p ₂ ρ $=$ ρ _{*fgh*.}

Pressure units. The SI unit for pressure is N/m², called *pascal* (Pa), while in Engineering, many other units are used, such as,

- bar: 1 bar≡1×10⁵ Pa= 100.0 kPa
- atm: 1 atm≡1.01325×10⁵ Pa=101.325 kP = 1.01325 bar
- $-$ psi (≡ lb_{*f*}/in²): 1 psi=6.8947×10³ Pa
- mm Hg: 1 mm Hg (at 0° C)=1.33×10² Pa
- in H₂O: 1 in H₂O (at 39.2°C)=2.491×10² Pa

Examples:

- 1. If p_{atm} = 756 mmHg, p_{abs} = 1358 mmHg, p_g = ? mmHg (602)
- 2. A gas is under 300 mmHg vacuum when $p_{atm} = 756$ mmHg, $p_{abs} = ?$ mmHg (456).

3. A gas is under normal atmospheric pressure when $p_{atm} = 756$ mmHg. $p_{abs} = ?$ mmHg (756), $p_g = ?$ mmHg (0).

3.3. Flow rate and velocity

Flow rate is the **amount of material flowing through a cross-sectional area in unit time**. The common flow rates in process engineering include the **mass flow rate (***m*: mass/time, kg/s), the **volumetric flow rate** (*Q*: volume/time, m^3 /s) and the **molar flow rate** (*N*moles/time, kg mol/s), their relationship is

$$
m = \rho Q
$$
, $N = m/M$

where ρ = density and M = molecular weight of the fluid.

The **velocity** of a fluid is the linear distance travelled per unit time by the fluid (length/time). The average velocity of a fluid through a duct of cross-section area $A: u = Q/A$. If the duct is a cylindrical pipe with an inside diameter D, $A = \pi (D/2)^2 = \frac{1}{4}\pi D^2$.

4. Mixture composition (Himmelblau, p26, p134; Felder, sec.4.7)

Concentration is the quantity of some solute in per fixed volume of a solvent, or solution, in

Fig. 4 A U-tube

a mixture of two or more components. It can be expressed by **mass per unit volume**, **moles per unit volume**, and, for very low concentrations, by **parts per volume (ppm)**, or for even lower by **parts per billion (ppb)**. The quantity of ppm or ppb is equivalent to a weight (mass) fraction for solids and liquids, and a mole or volume fraction for gases.

Mole and mass (weight) fractions: the mole (or mass) fraction of a component (*A*) in a mixture equals the moles (or mass) of *A* divided by the total number of moles (or the total mass) of the mixture. **Volume fraction** is often used for gases, which is equal to mole fraction at low pressures. In many cases the fractions are represented as percentages (mol %, wt% and $vol\%$.

Dry basis and wet basis composition: For mixtures containing water, the composition on a dry basis does not count the water content. For example,

- Air humidity: kg water/kg dry air (dry basis);
- Water content in solid: kg water/kg dry solid (dry basis), or given percent of water in the solid (wet basis).

Average molecular weight: The average molecular weight of a mixture containing two components, *A* and *B*, is given by

$$
\overline{M} = x_A M_A + x_B M_B
$$

where x_A and x_B denote the mole fractions and M_A and M_B molecular weights of components A and B, respectively.

Q: What is the average MWt of a mixture containing more than two components?

Molal units (Understand and remember!):

- mole $=$ g mol $=$ g mass/MWt
- $-$ kg mol = k mol = kg mass/MWt
- $-$ lb mol = lb mass/MWt

Since 1 kg =1000 g = 2.2 lb_m,

 $- 1$ kg mol = 1000 mol = 1000 g mol = 2.2 lb mol

(Note: lb_m means lb mass, but not lb mol)

Q: Does MWt have unit(s). If yes, what are they?

Ex. 150 kg of air $(21\% \text{ O2+ } 79\% \text{ N2}) = ?$ kg mol = lb mol?. MWt of O2 = 32, N2 = 28. Avg MWt of air = $0.21(32) + 0.79(28) = 28.84$; 1 kg = 2.2046 lb_m

 $n = 150 \text{ kg}/(28.84 \text{ kg/kg mol}) = 5.201 \text{ kg mol} (2.2046 \text{ lb}_m \text{mol/kg mol}) = 11.466 \text{ lb mol}$

5. Ideal gas law

An *ideal gas* or *perfect gas* is a gas that obeys the simple laws. The molecules of an ideal gas

are considered as

- (1) Being rigid spheres
- (2) Having no volume
- (3) Exerting no force on each other

Ideal gas law is valid for real gases at very low pressures, such as the air in the atmosphere, fuel gases and flue gases at low pressure. On the other hand, steam (pure water vapor) cannot be considered as an ideal gas while the water vapor in the air or a flue gas can.

The most important relationship for ideal gases is

pV=nRT (or *pQ= NRT*)

where $p =$ pressure, $V =$ volume (Q= volumetric flow rate), $T =$ temperature, $n =$ number of moles (N = molal flow rate), R = the gas law constant ($R = 8.314 \text{ m}^3$ -Pa/mol-K = 0.08206 m³atm/kg mol-K).

6. Meaningful and professional ways in writing numerical values

In addition to the bearing of a correct unit, the following points are of practical senses.

1) Use scientific expression for very long numbers.

Ex, 1246700→1.2467×10⁶; 0.0000345→3.45×10⁻⁵

2) Do not write too many decimal digits if they are insignificant to the number.

Ex. T = 298.1525 K \rightarrow 298.15 K (difference 0.0025 is negligible, less than 0.001%) or \rightarrow 298 K (the difference 0.1525 is only about 0.05%).

Ex. 3.16732 g → 3.167 g (difference 0.00032 is only about 0.01%)

In most calculations in this subject, you can omit the last few digits of a number in the final answer if they account for $\leq 1\%$ of the value.

Summary (Chapter 2 Terms and units)

- 1. The common unit systems, SI and English (or American Eng.), unit conversion; the rule and importance of dimensional consistency, dimensionless groups. Be especially familiar with the SI units for the basic dimensions (time, length, mass) and the important physical properties.
- 2. Definitions and units of important physical properties: density (ρ), specific volume (*v*), specific gravity (SpGr) and fluid viscosity (μ) .
- 3. Temperature and pressure scales and conversion; various flow rates and their conversion.
- 4. Representation and calculation of mixture composition and concentration, mass/vol., moles/vol., mole fraction, mass fraction, average molecular weight, and their conversion.
- 5. The definition of ideal gases and ideal gas laws, and gas law constant *R* and its units, and use the ideal gas law equation for calculation.

Important:

- Build up a strong awareness of the importance of units in expressing physical quantities. Missing the unit not only looses the value but also the meaning of the quantity!

- Build up a strong sense of dimension consistency in writing equations.

Examples

1. Unit conversion

1) Density of water
$$
\rho = 1000 \text{ kg/m}^3
$$
 (at 4°C) to g/L and lb/ft³

$$
\rho = \frac{1000 \text{ kg} [1000 \text{ g}]}{m^3} \frac{1 \text{ m}^3}{1 \text{ kg} } = 1000 \text{ g/L} = \left[\frac{1000 \text{ kg} [2.2046 \text{ lb}]}{m^3} \left(\frac{1 \text{ m}}{3.2808 \text{ ft}}\right)^3\right] = 62.43 \text{ lb/ft}^3
$$

2) Viscosity of water (at 20 °C) μ = 1.005 cp = 1.005 ×10⁻³ Pa-s to lb/ft-s 1.005×10^{-3} Pa-s = 1.005×10^{-3} kg/m-s $=1.005 \times 10^{-3}$ (2.2046 lb)/3.2808ft-s = 6.753 $\times 10^{-4}$ lb/ft-s

3) Mass flow rate water $m = 1$ kg/s to kg/h, and to molar flow rate in kg mol/h and volumetric flow rate in m³/min (assuming $\rho = 1000 \text{ kg/m}^3$)

$$
m = 1 \text{ kg/s} = \frac{1 \text{ kg}}{s} \left(\frac{3600 \text{ s}}{1 \text{ h}} \right) = 3600 \text{ kg/h}
$$

Molar flow rate N = (3600 kg/h) (1 kg mol H2O/18.02 kg) = 199.78 kg mol/h Volumetric flow rate $Q = m/\rho =$ min . / / 60 $3.6 \, m^3$ 1 1000 3600 kg / $h = 3.6 \ m^3$ 3 *h h m kg m* $\frac{kg/h}{\frac{m^3}{2}} = \frac{3.6 \, m^3}{2.0 \, \text{m/s}} = 0.06 \, \text{m}^3/\text{min}$

2. Dry basis and wet basis composition. Air humidity H and solid moisture content X are often expressed in dry basis, H as kg water/kg dry air, and X as kg water/kg dry solid. How to convert these content based on the total weight of air or solid (total including both water and the dry solid)?

Ans: H kg water/kg dry air is equivalent to H kg water/ $(H + 1)$ kg total air and X to $X/(X+1)$ total solid.

3. Dimension and units

The reaction rate for the gas-phase reaction $2NO+O_2 \rightarrow 2 NO_2$ is represented by (according to Fogler), $r = -\frac{dC_{N0}}{dt} = kC_{N0}^2C_{O2}$. If concentration is in mol/L and time in s, derived the units for *r* and *k*.

Solution: $[r] = [C]/[t] = \text{mol/L-s}$

 $mol/L-s = [k] (mol/L)²(mol/L), [k] = (mol/L-s)/(mol/L)²(mol/L) = (mol/L)⁻² s⁻¹$