Introduction to Chemical Engineering Calculations

Md Khairul Islam (Ph.D.)
Applied Chemistry & Chemical Engineering
Rajshahi University

Importance of ChE calculations

Chemical engineers use quantitative analysis to design and analyze processes. These calculations are essential for-

- Designing chemical reactors and process equipment
- Determining flow rates, compositions, and energy requirements
- Ensuring safety and efficiency in industrial processes
- Scaling laboratory processes to industrial production

All chemical engineering calculations are based on fundamental conservation laws: (mass conservation; energy conservation; and momentum conservation.

Dimensions and Units

- Dimensions are our basic concepts of measurement such as length, time, mass, temperature, and, so on.

- Units are the means of expressing the dimension such as feet or centimeters for length and seconds or hours for time.

- A ***dimension*** is a measure of a physical variable (without numerical values), while a ***unit*** is a way to assign a number or measurement to that dimension.

- For example, length is a dimension, but it is measured in units of feet (ft) or meters (m).

Dimensions and Units

The two most commonly used systems of units:

- SI system of units.
- AE, or American Engineering system of units

Dimensions and their respective units are classified as:

- Fundamental (or basic) dimensions /units are those that can be measured independently and are sufficient to describe essential physical quantities.
- Derived dimensions and units are those that can be developed in terms of the fundamental dimensions and units.

TABLE 1.1 SI Units Encountered in This Book

Physical Quantity	Name of Unit	Symbol for Unit*	Definition of Unit
	Basic SI Units		
Length	metre, meter	m	
Mass	kilogramme, kilogram	kg	
Time	second	s	
Temperature	kelvin	K	
Molar amount	mole	mol	
	Derived SI Units		
Energy	joule	J	$kg \cdot m^2 \cdot s^{-2} \rightarrow Pa \cdot m^3$
Force	newton	N	$kg \cdot m \cdot s^{-2} \rightarrow J \cdot m^{-1}$
Power	watt	W	$kg \cdot m^2 \cdot s^{-3} \rightarrow J \cdot s^{-1}$
Density	kilogram per cubic meter		$kg \cdot m^{-3}$
Velocity	meter per second		$m \cdot s^{-1}$
Acceleration	meter per second squared		$m \cdot s^{-2}$
Pressure	newton per square meter, pascal		$N \cdot m^{-2}$, Pa
Heat capacity	joule per (kilogram · kelvin)		$J \cdot kg^{-1} \cdot K^{-1}$
	Alternative Units		
Time	minute, hour, day, year	min, h, d, y	
Temperature	degree Celsius	°C	
Volume	litre, liter (dm^3)	L	

TABLE 1.2 American Engineering (AE) System Units Encountered in This Book

Physical Quantity	Name of Unit	Symbol
	Some Basic Units	
Length	foot	ft
Mass	pound (mass)	lb_m
Time	second, minute, hour, day	s, min, h (hr), day
Temperature	degree Rankine or degree Fahrenheit	°R or °F
Molar amount	pound mole	lb mol
	Derived Units	
Force	pound (force)	lb_f
Energy	British thermal unit, foot pound (force)	Btu, $(ft)(lb_f)$
Power	horsepower	hp
Density	pound (mass) per cubic foot	lb_m/ft^3
Velocity	feet per second	ft/s
Acceleration	feet per second squared	ft/s^2
Pressure	pound (force) per square inch	$lb_f/in.^2$, psi
Heat capacity	Btu per pound (mass) per degree F	$Btu/(lb_m)(°F)$

Operations with Units

- **Addition, Subtraction, Equality**

  You can add, subtract, or equate numerical quantities only if the associated units of the quantities are the same. Thus, the operation

  - *5* kilograms + 3 joules $\longrightarrow$ –/+ cannot be carried out
  - 10 pounds + *5* grams $\longrightarrow$ –/+can be performed *only* after the units are transformed to be the same.

- **Multiplication and Division**

  You can multiply or divide unlike units at will such as

  SO(kg)(m)/(s)

  but you cannot cancel or merge units unless they are identical.

Dimensional Homogeneity

A basic principle states that equations must be dimensionally consistent which means each term in an equation must have the same net dimensions and units as every other term to which it is added, subtracted, or equated.

$$\Delta E + \Delta(P\bar{V}) + \frac{\Delta v^2}{2} + g\,\Delta z = Q - \dot{W}_s$$

In the absolute system, the dimensions of the terms are mass M, length L, time Θ, energy ML^2/Θ^2, force ML/Θ^2, volume L^3, and area L^2. The dimensions of the terms in Eq. (3.49) are, therefore,

$$\frac{\mathrm{ML}^2/\Theta^2}{\mathrm{M}} + \frac{\mathrm{ML}/\Theta^2}{\mathrm{L}^2}\frac{\mathrm{L}^3}{\mathrm{M}} + \left(\frac{\mathrm{L}}{\Theta}\right)^2 + \frac{\mathrm{L}}{\Theta^2}\mathrm{L} = \frac{\mathrm{ML}^2/\Theta}{\mathrm{M}} - \frac{\mathrm{ML}^2/\Theta^2}{\mathrm{M}}$$

Canceling dimensions gives

$$\frac{\mathrm{L}^2}{\Theta^2} + \frac{\mathrm{L}^2}{\Theta^2} + \frac{\mathrm{L}^2}{\Theta^2} + \frac{\mathrm{L}^2}{\Theta^2} = \frac{\mathrm{L}^2}{\Theta^2} - \frac{\mathrm{L}^2}{\Theta^2}$$

Dimensional Homogeneity

If, dimension F is used for force and E is for energy then the energy balance equation becomes

$$\frac{E}{M} + \frac{F}{L^2}\frac{L^3}{M} + \left(\frac{L}{\Theta}\right)^2 + \frac{L}{\Theta^2}L = \frac{E}{M} - \frac{E}{M}$$

This is dimensionally inconsistent. To achieve dimensional consistency, it is necessary to use dimensional constant relating to the redundant dimension-

$$g_c = \frac{ML}{\Theta^2 F}$$

$$J = \frac{FL}{E}$$

Dimensional Homogeneity

$$\mathbf{F}g_c = \frac{\mathbf{ML}}{\Theta^2}$$

and

$$\mathbf{E}J = \mathbf{FL}$$

Combining Eqs. (3.52*a*) and (3.53*a*) gives

$$\mathbf{E}Jg_c = \frac{\mathbf{ML}^2}{\Theta^2}$$

The right-hand side of Eq. (3.52*a*) is the correct dimensions of force in the absolute system; therefore, $\mathbf{F}g_c$ should be used in Eq. (3.51) instead of **F**. Similarly, Eq. (3.54) shows that energy should be $\mathbf{E}Jg_c$ instead of **E**. With these corrections Eq. (3.51) becomes

$$\frac{\mathbf{E}Jg_c}{\mathbf{M}} + \frac{\mathbf{F}g_c}{\mathbf{L}^2}\frac{\mathbf{L}^3}{\mathbf{M}} + \left(\frac{\mathbf{L}}{\Theta}\right)^2 + \frac{\mathbf{L}}{\Theta^2}\mathbf{L} = \frac{\mathbf{E}Jg_c}{\mathbf{M}} - \frac{\mathbf{E}Jg_c}{\mathbf{M}}$$

This equation can be shown to be dimensionally consistent by combining Eqs. (3.52*a*) and (3.54) with it. For this system of dimensions Eq. (3.49) becomes

$$\Delta EJg_c + \Delta(P\bar{V})g_c + \frac{\Delta v^2}{2} + g\,\Delta z = QJg_c - W_sJg_c$$

Dimensionless group

- A groups of symbols, may be put together, have no net units. Such collections of variables or parameters are called dimensionless groups.
- These numbers eliminate units and reduce the number of variables, allowing engineers to compare different systems and extrapolate results from one scale to another. Additionally, they relate dimensionless numbers to each other and to important output variables.
- One example is the Reynolds number (group) arising in fluid mechanics.

$$\text{Reynolds number} = \frac{Dv\rho}{\mu} = N_{RE}$$

Unit conversion

- **Example:** If a plane travels at twice the speed of sound (assume that the speed of sound is 1100 ft/s), how fast is it going in miles per hour?

  - Solution: $$2 \times \frac{1100\ \text{ft}}{\text{s}} \left| \frac{1\ \text{miles}}{5280\ \text{ft}} \right| \frac{60\ \text{s}}{1\ \text{min}} \left| \frac{60\ \text{min}}{1\ \text{hr}} \right.$$

- **Example:** (a) Convert 2 km to miles; (b) Convert 400 in3/day to cm3/min.

- Solution: (a)

$$\frac{2\ \text{km}}{} \left| \frac{1\ \text{mile}}{1.61\ \text{km}} \right. = 1.24\ \text{mile}$$

(b)

$$\text{(b)}\quad \frac{400\ \text{in.}^3}{\text{day}} \left| \left(\frac{2.54\ \text{cm}}{1\ \text{in.}}\right)^3 \right| \frac{1\ \text{day}}{24\ \text{hr}} \left| \frac{1\ \text{hr}}{60\ \text{min}} \right. = 4.55\,\frac{\text{cm}^3}{\text{min}}$$

Unit conversion

Example: A semiconductor (ZnS) with a particle diameter of 1.8 nanometers. Convert this value to: (a) dm (decimeters) (b) inches.

Solution: (a) $\dfrac{1.8\ \text{nm}}{}\left|\dfrac{10^{-9}\ \text{m}}{1\ \text{nm}}\right|\dfrac{10\ \text{dm}}{1\ \text{m}} = 1.8 \times 10^{-8}\ \text{dm}$

(b) $\dfrac{1.8\ \text{nm}}{}\left|\dfrac{10^{-9}\ \text{m}}{1\ \text{nm}}\right|\dfrac{39.37\ \text{in.}}{1\ \text{m}} = 7.09 \times 10^{-8}\ \text{in.}$

Example: Water has a density of 62.4 lbm /ft³. How much does 2.000 ft³ of water weigh at sea level and 45° latitude?

The mass of water $m = \left(62.4\ \dfrac{\text{lb}_m}{\text{ft}^3}\right)(2\ \text{ft}^3) = 124.8\ \text{lb}_m$

The weight of water $W = (124.8\ \text{lb}_m)g\left(\dfrac{\text{ft}}{\text{s}^2}\right)\left(\dfrac{1\ \text{lb}_f}{32.174\ \text{lb}_m\cdot\text{ft/s}^2}\right)$

At sea level $g = 32.174\ \text{ft/s}^2$, so that $W = 124.8\ \text{lb}_f$.

Unit conversion

Example: What is the potential energy in (ft)(lb1) of a 100 lb drum hanging 10 ft above the surface of the earth with reference to the surface of the earth?

Solution: Potential Energy= *mgh*

$$P = \frac{100\ \text{lb}_m}{} \left| \frac{32.2\ \text{ft}}{\text{s}^2} \right| \frac{10\ \text{ft}}{} \left| \frac{(\text{s}^2)(\text{lb}_f)}{32.174(\text{ft})(\text{lb}_m)} \right. = 1000\ (\text{ft})(\text{lb}_f)$$

Example: Experiments show that 1 μg mol of glucoamylase in a 4% starch solution results in a production rate of glucose of 0.6 μg mol/(ml)(min). Determine the production rate of glucose for this system in the units of lb mol/(ft^3)(day).

Solution:

$$\frac{0.6\ \mu\text{g mol}}{(\text{mL})(\text{min})} \left| \frac{1\ \text{g mol}}{10^6\ \mu\text{g mol}} \right| \frac{1\ \text{lb mol}}{454\ \text{g mol}} \left| \frac{1000\ \text{mL}}{1\ \text{L}} \right| \frac{1\ \text{L}}{3.531 \times 10^{-2}\ \text{ft}^3} \left| \frac{60\ \text{min}}{\text{hr}} \right| \frac{24\ \text{hr}}{\text{day}}$$

$$= 0.0539 \frac{\text{lb mol}}{(\text{ft}^3)(\text{day})}$$

Basis: 1 min

Unit conversion

Example: Convert 25 liter-atm to Btu

Solution-

$$25\ liter - atm \times \frac{1000\ cm^3}{1\ liter} \times (\frac{1\ ft}{30.4\ cm})^3 \times \frac{14.7\ lb_f/inch^2}{1\ atm} \times (\frac{12\ inch}{1\ ft})^2 \times \frac{1\ Btu}{778\ ft\text{−}lb_f}$$

$$= 25 \times \frac{1000}{1} \times (\frac{1}{30.4})^3 \times \frac{14.7}{1} \times (\frac{12}{1})^2 \times \frac{1}{778}$$

$$liter - atm \times \frac{cm^3}{liter} \times (\frac{ft}{cm})^3 \times \frac{lb_f/inch^2}{atm} \times (\frac{inch}{ft})^2 \times \frac{Btu}{ft\text{−}lb_f}$$

$$= 2.52\ Btu$$

$1\ atm = 14.7\ lb_f/inch^2$

$1\ liter = 1000cm^3$

$1\ ft = 12\ inch = 30.4\ cm$

$1\ Btu = 778ft - lb_f$

Validation of Problem Solutions

- Repeat the calculations, possibly in a different order.
- Start with the answer and perform the calculations in reverse order.
- Review your assumptions and procedures. Make sure two errors do not cancel each other.
- Compare numerical values with experimental data or data in a database (handbooks, the Internet, textbooks).
- Examine the behavior of the calculation procedure. For example, use another starting value and check that the result changed appropriately.
- Assess whether the answer is reasonable given what you know about the problem and its background.

Significant Figures

The significant figures of a given number are those significant or important digits, which convey the meaning according to its accuracy. For example, 6.658 has four significant digits. These substantial figures provide precision to the numbers.

Number	Number of Significant digits/figures
45	Two
0.046	Two
7.4220	Five
5002	Four
3800	Two

Significant Figures

- All non-zero digits are significant. 198745 contains six significant digits.
- All zeros that occur between any two non zero digits are significant. For example, 108.0097 contains seven significant digits.
- All zeros that are on the right of a decimal point and also to the left of a non-zero digit is never significant. For example, 0.00798 contained three significant digits.
- All zeros that are on the right of a decimal point are significant, only if, a non-zero digit does not follow them. For example, 20.00 contains four significant digits.
- All the zeros that are on the right of the last non-zero digit, after the decimal point, are significant. For example, 0.0079800 contains five significant digits.
- All the zeros that are on the right of the last non-zero digit are significant if they come from a measurement. For example, 1090 m contains four significant digits

Significant Figures

Not significant:
zero for "cosmetic" purpose

Not significant:
zeros used only to locate the decimal point

Significant:
all zeros between nonzero numbers

0 . 0 0 4 0 0 4 5 0 0

Significant:
all nonzero integers

Significant:
zeros at the end of a number to the right of decimal point

Significant Figures

- When you add or subtract numbers, keep the same number of decimal places as the factor with the least amount.

Example: 1.234 + 5.67 =6.90 Not 6.904

- When you multiply or divide numbers, keep the same number of significant figures as the factor with the least number of significant figures.

Example: 1.2 x 4.56 = 5.5 Not 5.472

1 **What are the significances of unit conversion for engineering calculation?** 1.5

2. **Convert the following quantities to the unit indicated-** 3

   (i)Density of 1g/cm^3 to lb/ft^3

   (ii)Pressure of 1 atm to dynes/cm^2

   (iii)Heat capacity of 1 joule/g°C to Btu/lb°F

3. **Mention the number of significant digits of the following values-** 3

   500032; 0.0004500; 0.0080530; 0.0650; 0.00500; 705.0L.