1

Industrial Processing and Basic Principles

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Pharmaceutical engineering is concerned with the study of industrial processes in which raw materials are changed or separated into pharmaceutically useful products such as drugs and excipients. A wide variety of processes are involved in these conversions. Some of them are as follows.

1. Production of dosage forms : Conversion of drugs (chemicals as raw materials) into medicines (*dosage forms*), which are suitable for use by the patient. Example is conversion of diclofenac sodium into dosage forms such as tablets, capsules, suspensions and injections.

2. Production of bulk drugs : Chemicals (raw materials) are converted into drugs. For example, salicylic acid is acetylated to obtain acetylsalicylic acid (aspirin). This area is known as production of *Bulk Drugs*. Conversion of chemicals into intermediates, which in turn are used for production of drugs in commercial scale, is also included in this area.

3. Production of antibiotics : Manufacture of drugs (antibiotics) using microbes with the aid of precursors is another area of interest to the pharmacist. This area is known as *fermentation technology*. For example, penicillin G is produced using *Penicillium chrysogenum* with the aid of precursor, phenylacetic acid.

4. Production of biologicals : Extraction of drugs from animals, plants and minerals from native raw materials into purified (or semi-purified) products are of interest to the pharmacist. Some examples are vaccines, insulin, streptokinase and recombinant DNA technology products.

Each process is developed systematically from a laboratory scale to pilot scale and finally to an industrial scale. In each case, process is undertaken by employing a number of equipment. The areas of interest with reference to equipment are:

- design
- fabrication
- assembly
- operation
- maintenance

Similarly, each process has to be followed scrupulously in terms of:

- effectivity
- efficiency
- validity
- safety
- economy

Effectiveness refers to the quality of what is to be actually accomplished. *Efficiency* means accomplishing tasks with a minimum of wasted material, time and money. In the popular management cliché, efficiency is doing things right, while effectiveness is doing right things.

Validation is defined as a procedure that demonstrates the ability of consistently producing a product with the established specifications under ideal conditions.

Safety refers to the protection of products, personnel, factory etc. Prevention of accidents and protection from fire constitute important aspects. Sufficient care should be exercised so that human factor is removed from the hazards by making protection a permanent and automatic.

Economy refers to the protection of factory from financial problems. The industrial activity essentially involves the conversion of raw materials into value added products. The steps are initiated for the optimization of parameters for an operation and process, so that economy works out for the factory as well as customer (or consumer). Standard Operating Procedures (SOPs) are helpful to obtain a quality product coupled with economy.

Therefore, a broad understanding of the basic principles involved in a process, knowledge about the construction, working and skills in handling them are of vital importance. This chapter provides the basic information and prerequisites that are necessary for understanding pharmaceutical engineering.

UNIT OPERATIONS AND UNIT PROCESSES

Normally, every process involves a series of steps. Each step is performed individually. This approach is an economical way of organizing a given task.

Unit Operations

Each chemical process frequently consists of a fewer number of distinct individual steps. Each step is called *unit operation*.

Each unit operation is based on one type of scientific principle. A few examples of unit operations and underlying principles are listed below.

Drying : It is a unit operation used to remove liquid or moisture from solids by evaporation with the aid of heat. For example, drying process is employed to remove excess moisture (above equilibrium moisture content) from the wet granules in the production of tablets.

Size reduction : This is a unit operation in which drugs (vegetable or chemical origin) are reduced to smaller pieces, coarse particles or fine powder. This process is extensively used in the manufacture of talcum powders and tooth powders (cosmetic industry).

Distillation : It is a unit operation of converting liquid into vapour by heating and reconverting vapour again into liquid by condensing the vapour. This unit operation is used for obtaining essential oils from various parts of the plants. Example is lemon-grass oil (perfume industry).

Evaporation : It is a unit operation which involves free escape of vapour from the surface of a liquid below its boiling point. For example, evaporation technique is extensively used for concentrating the syrup in the manufacture of sugar (sugar industry).

The **advantage** is that each unit operation is a common technique and employed in diverse chemical and pharmaceutical industries. For example, the operation of mass transfer is involved in humidification, evaporation, distillation, extraction and drying. The unit operation of drying is used in the following industries.

(1) **Pharmaceutical industry :** In the production of tablets, the powdered mass is converted into wet mass, which is subsequently dried in order to obtain free flowing dry granules.

In the manufacture of herbal drug extracts, a large number of plants are used. The plant extracts are dried in order to extend the shelf life. Otherwise, the product may deteriorate. For example, in the preparation of belladonna dry extract IP, liquid extract of belladonna is dried completely. Otherwise it gets deteriorated.

(2) **Food industry :** Grapes, cashew, almonds and other types of fruits are dried to obtain dry fruits. These products have extended storage life.

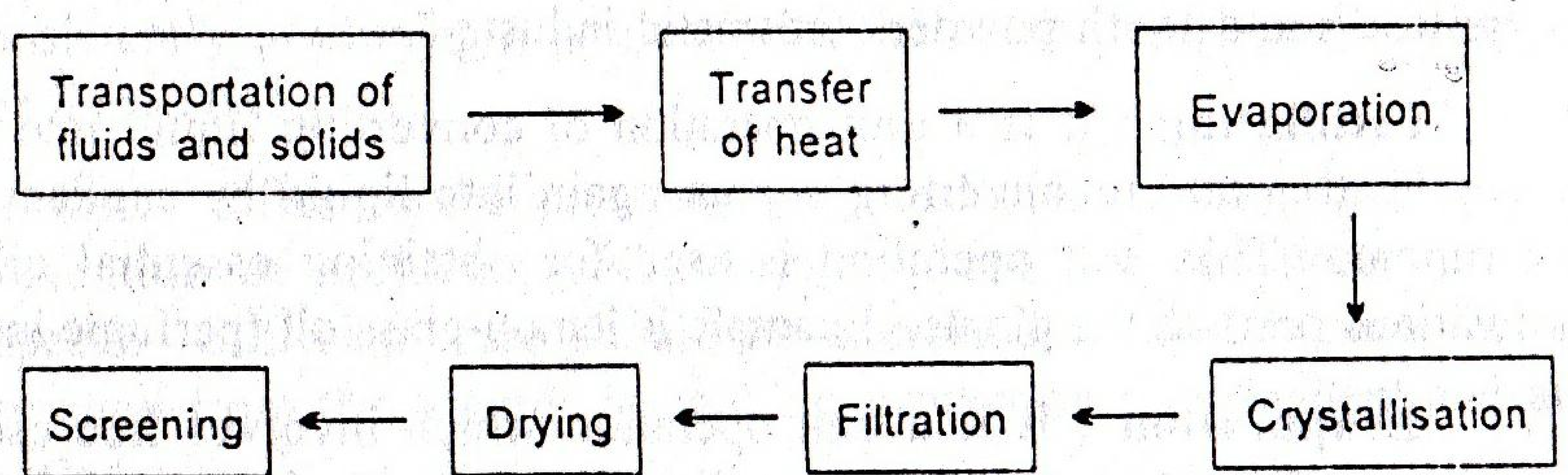
(3) **Sugar industry :** The crystals of sugar are dried to remove residual water, so that the sugar will be dry and free flowing.

Unit operations are based on both science and experience. The theory and practice must be combined judiciously for achieving proficiency in handling equipment.

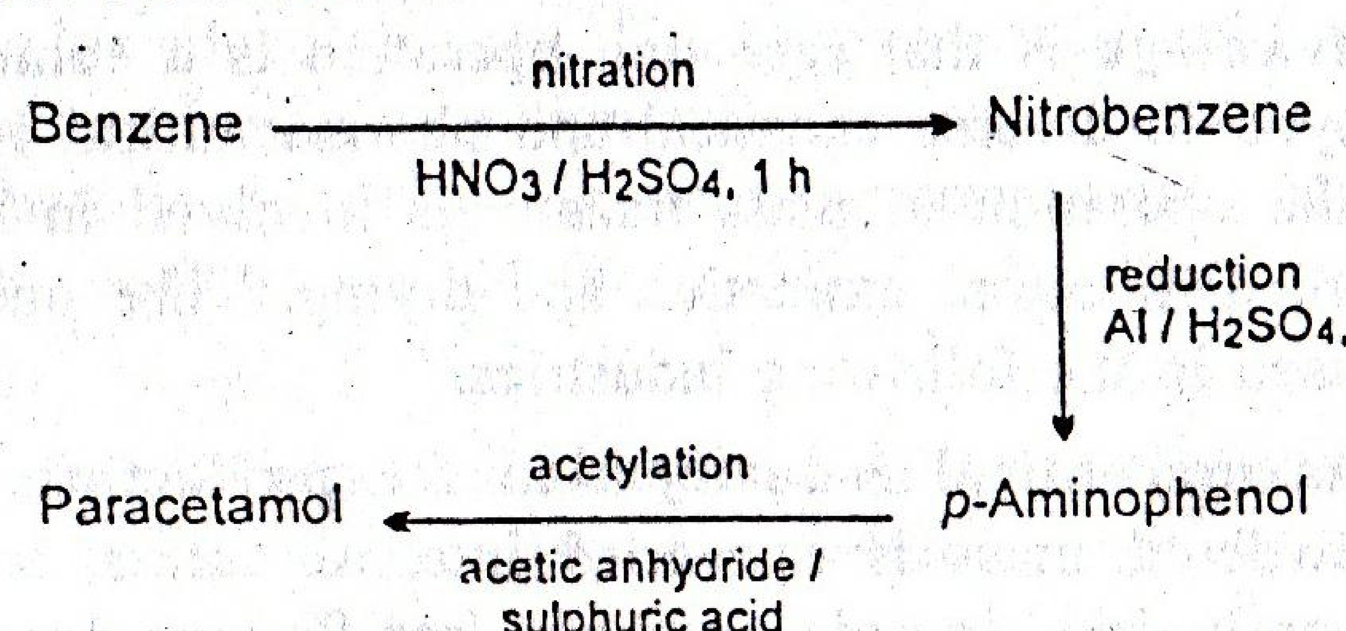
Unit Process

Unit process is defined as the one in which several unit operations are combined in a sequence to achieve the objectives of a chemical or physical process.

Unit process-Physical process : Consider the example of manufacture of common salt. The unit operations involved are:

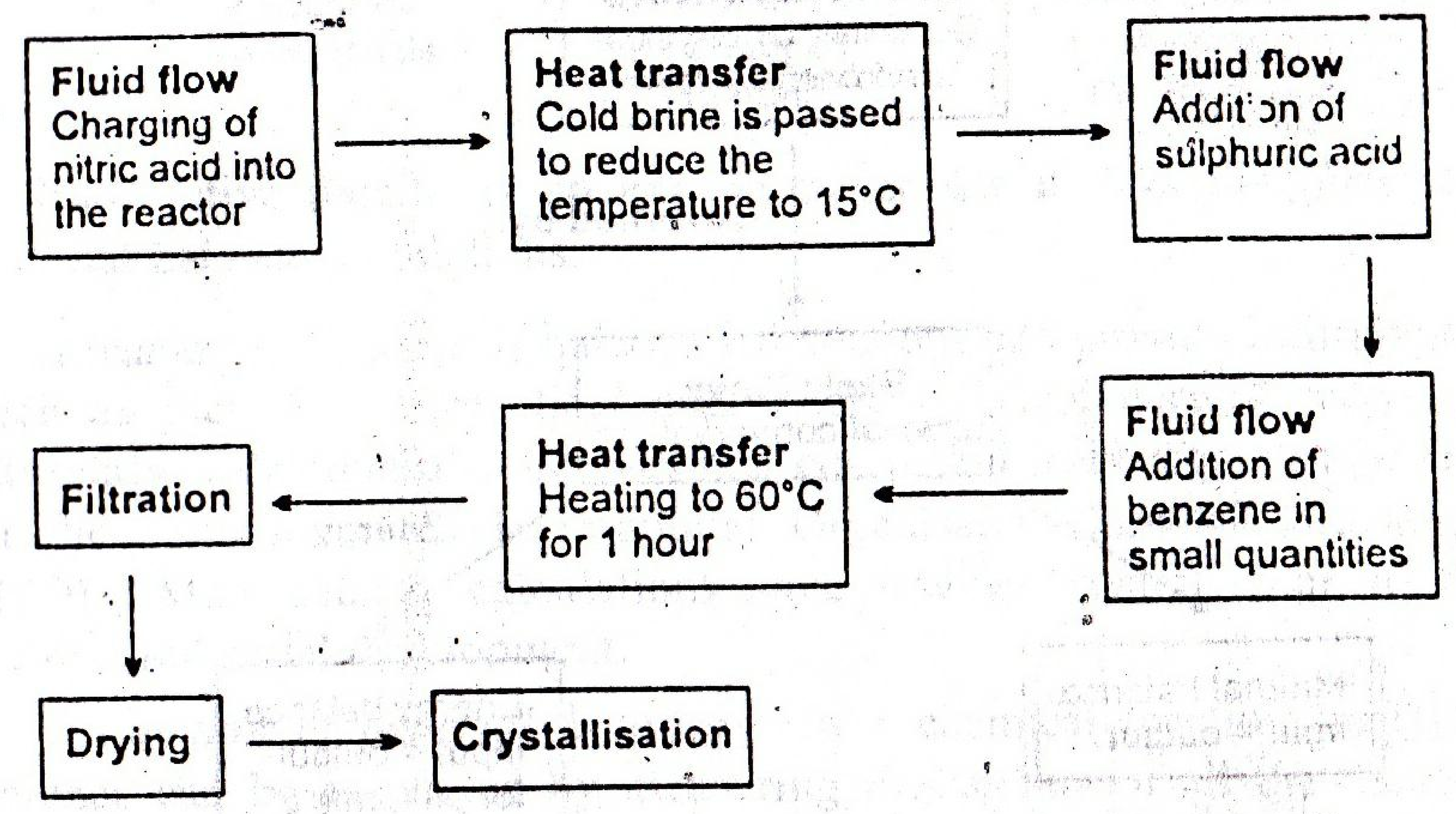


Unit process—Chemical process : Consider the production of paracetamol from benzene.



Sequence of reactions for the production of paracetamol (or acetaminophen).

In the above process, three unit processes are involved. These are nitration, reduction and acetylation. Each unit process is in turn made of a number of unit operations. For example, in the nitration of benzene to nitrobenzene, the unit operations involved are:



These examples illustrate that unit operations are largely used to conduct the physical steps such as:

1. Preparation of the reactants,
2. Separation and purification of the products,
3. Recycling of the unconverted reactants,
4. Controlling of the energy transfer into or out of the chemical reactor.

Thus, several steps are carried in a sequential order to achieve a process efficiently and economically.

UNIT OPERATIONS—SCIENTIFIC FOUNDATIONS

A large number of unit operations are simultaneously handled in a chemical process. Hence, the knowledge of the elementary physical and chemical laws (Figure 1-1) is essential for the application of scientific principles and techniques. Some of these laws are:

Basic laws: Laws of conservation of matter.
Laws of conservation of energy.

Special laws: Universal gas laws (Ideal gas equation).
Dalton's law of partial pressures.

Special laws are discussed in detail in different books mentioned in bibliography. The basic laws are highlighted below.

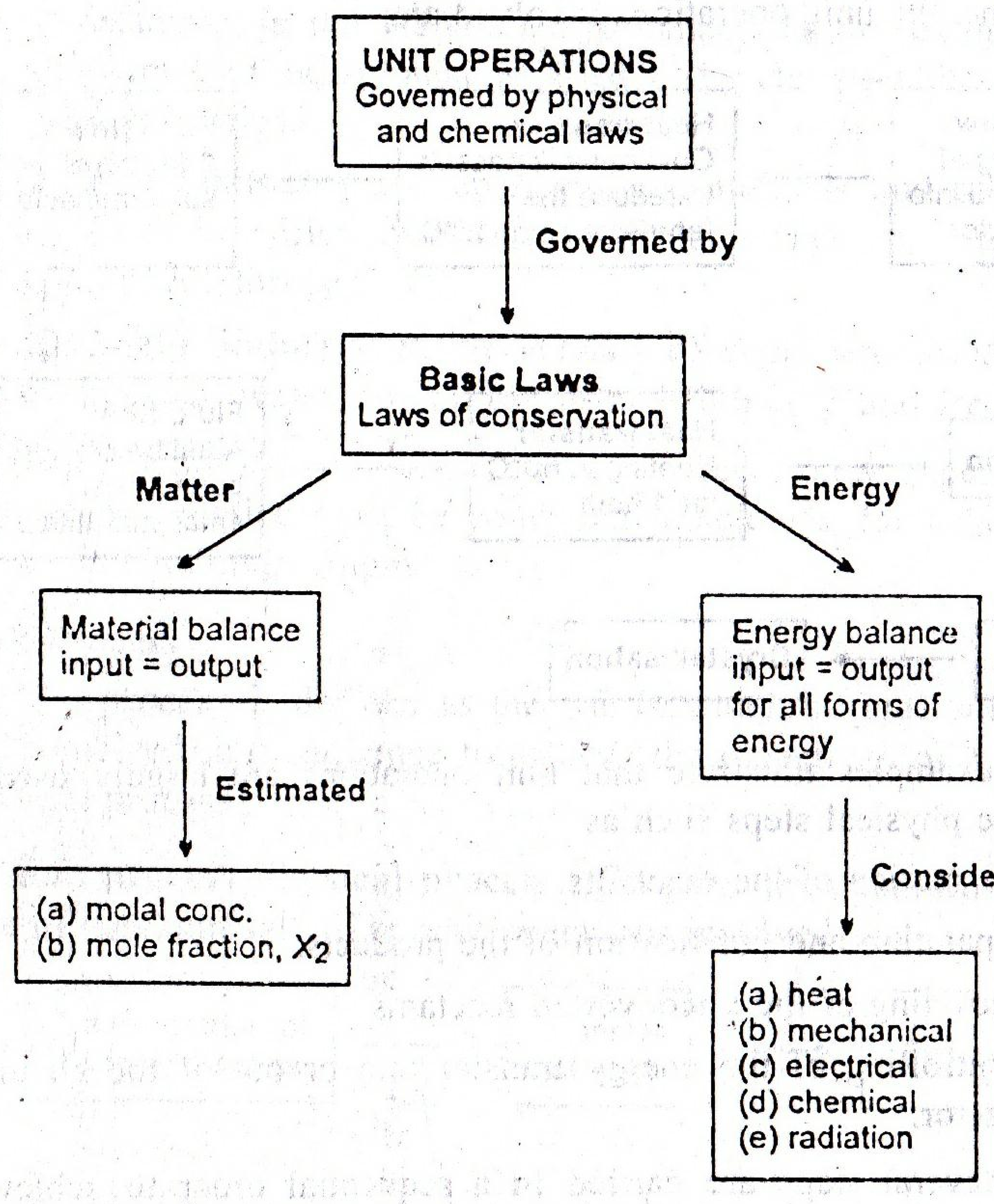


Figure 1-1. Scientific foundations in unit operations. Basic laws are included.

Basic Laws

The general law of conservation can be applied to any process. It is employed in engineering in the form of:

(a) Material balance
(b) Energy balance

Material balance : *The law of conservation of matter* states that material cannot be destroyed or created, it can be changed from one form to another.

In other words, the material entering a process must either accumulate or leave the process. The given input must be accounted for an output. The principle of material balance can be applied to an equipment, or to the entire process or any part of it. A simple account of material balance

INPUT	=	OUTPUT		
Amount of raw materials		Amount of changed materials	+	Amount of unchanged materials

Radioactive process is an exception because it does not obey the material balance calculations.

Advantages : The mass balance calculations can provide information such as yield value (practical and theoretical) and percent recovery. Currently, validation of processes and equipment has become important in the certification of International Organisation for Standardisation (ISO). Mass balance calculations have assumed central place in the current industrial development.

Estimation of material balance : In a chemical reaction, material balance can be accounted by measuring the amount of all the components (constituents). Normally, the amount is expressed in concentration units; moles/litre, molal units, mole fraction units, % w/v, % w/w etc. Some of them are reported for ready reference.

Mole : In a chemical reaction, the molecular unit is *gram mole* or *pound mole*. Some important expressions are molal units and mole fraction units.

In the mass balance calculations, mole is a better term and used frequently. For an individual component, mole is defined as quantity of that substance whose mass is numerically equal to its molecular weight.

$$\textit{Gram-moles of a substance} = \frac{\text{mass in grams}}{\text{molecular weight}} \qquad (1)$$

These values are useful while selecting the amount of each ingredient to be added to the reaction mixture based on the stoichiometric equation and coefficients. For example, x grams of oxygen gas has been mathematically expressed as:

$$\textit{Number of moles} = \frac{x \text{ grams of oxygen}}{\text{molecular weight of oxygen}} = \frac{x \text{ grams}}{32}$$

Average molecular weight: When a mixture of substances is involved in a reaction, the average molecular weight of the mixture may be written as:

$$\text{Average molecular weight of mixture, } m = \frac{W_a + W_b + W_c + \ldots\ldots}{\frac{W_a}{M_a} + \frac{W_b}{M_b} + \frac{W_c}{M_c} + \ldots\ldots} \quad (2)$$

where W_a, W_b, W_c etc. are the weights of individual components a, b, c. etc. M_a, M_b, M_c etc. are the molecular weights of components a, b, c. etc.

Molality : For individual components, molality is expressed as:

$$\text{Molality, } m = \frac{\text{number of moles of substance}}{\text{number of kg of medium (solvent)}} \quad (3)$$

The unit is mol kg^{-1}. It is designated as m. Molality (molal) notation is frequently used in theoretical studies. The **advantages** are enumerated below.

(a) It does not change with temperature, i.e., contraction or expansion of a liquid with temperature does not affect the calculations.

(b) The weight of solvent (reaction medium) is considered. Volume has no influence, since it is not precisely known always.

Mole fraction : For individual component, mole fraction is expressed as:

$$\text{Mole fraction of A, } X_A = \frac{\text{number of moles of one constituent}}{\text{total number of moles of all constituents}}$$

It is designated as X. One constituent may be solute. Total number of moles of all the constituents refers to moles of solutes and solvents. It is in general notations as:

$$\text{Mole fraction of A, } X_A = \frac{\frac{W_a}{M_a}}{\frac{W_a}{M_a} + \frac{W_b}{M_b} + \frac{W_c}{M_c}}$$

$$= \frac{n_a}{n_a + n_b + n_c + \ldots} \quad (4)$$

where n_a, n_b, n_c etc., are the number of moles of individual components a, b, c, etc.

The sum of the mole fractions of all components must be equal to unity. Mole fraction is used frequently in experiments involving theoretical considerations. The **advantage** of mole fraction notaion is that it expresses the relationship between the reactants and other components in a simple and direct way.

Energy balance : *Energy* is the capacity to exert a force through a distance and manifests itself in various forms.

The unit of energy in SI system is J (Joule). The energy per unit mass is known as *specific energy*, which has the unit of J/kg. Engineering processes involve: (a) conversion of energy from one form to another (b) transfer of energy from place to place (c) storage of energy in various forms utilizing a working substance. The first law of thermodynamics is a statement of conservation of energy. It expresses the fact that energy cannot be created or destroyed, though energy can be transported from one kind to another.

The *law of conservation of energy* states that the energy output must be same as the energy input in a chemical process.

The energy balance equation must include all types of energies.

* heat * mechanical * electrical

* chemical * radiation

When one kind of energy is destroyed or consumed, an equal amount of another kind must be formed.

Applications : The principle of conservation of energy is applied in a number of instances. A few of them are mentioned here.

(1) In the study of fluid flow, Bernoulli's theorem is applied, which is a special case of the law of conservation of energy.

(2) Energy is converted from one form to another. This principle is used in the working of a pump wherein kinetic energy is converted into pressure head for pumping the liquids.

(3) Energy losses due to friction can be accounted, while a fluid is flowing through pipes. It is also helpful for adopting suitable measures to reduce losses.

(4) Since efficiency and economy are important parameters for any process (chemical or physical), energy calculations and balancing have assumed importance. When energy is obtained from non-renewable sources, balancing of energy will be a critical factor.

Some Basic Concepts

Rate of a process or reaction : The rate of a reaction can be understood by studying the time course changes in the concentration. In general, rate is expressed mathematically as a differential equation:

$$\text{Rate of reaction} = \frac{dQ}{dt} = \frac{dF}{R} = \frac{\text{driving force}}{\text{resistance}} \quad (5)$$

where Q = quantity being transferred or reacted
t = time
F = driving force
R = resistance

According to equation (5), the rate at which a system approaches equilibrium may be expressed as the combined effect of two factors. These are:

(*a*) *Potential factor* : It indicates the driving force necessary to make (proceed) the reaction.

(*b*) *Resistance factor* : It indicates the capacity to impede the speed for a given potential.

In the example of heat transfer from the hotter end of the iron rod to the colder end, the driving force is the difference in temperature (ΔT). At the same time, iron also offers certain amount of resistance to heat flow, on account of poor thermal conductivity.

Steady state and unsteady state : In a system, if the operating conditions are varying with time, then such a system is said to be in *unsteady state* or *transient state*.

For example, consider a tank of cold water. A coil in which constant pressure of steam is maintained is immersed in the tank. During the heat transfer through the coil, the operating conditions such as temperature difference between the coil and water do not remain same with time. Similarly, thermal resistance between the coil and water changes with time.

A system is said to be at *steady state*, if the conditions do not vary with time..

For example, consider water in a pipe is flowing under two conditions. (A) Water entering the tank at constant temperature and flow rate. (B) A jacket in which steam is maintained at constant temperature surrounds the pipe. Condition may vary from section to section along the pipe, but at any one cross section, it does not vary with time.

DIMENSIONS, UNITS, SYSTEMS AND INTER-CONVERSIONS

For the purpose of measurement (dimensions), three systems have been used, namely:

Cgs system (centimetre-gram-second)—Also known as metric system

Fps system (foot-pound-second)—Also known as British system

Mks or SI (metre-kilogram-second)—Modern system

The basic quantities identified for this purpose are length, mass, time etc. These are expressed in various ways in different systems. Some of the important principles in dimensions are given in Figure 1-2.

The units mentioned in any system for expressing the physical quantities are known as *fundamental units* or *primary units*.

For example, length is expressed as centimetre in cgs system, foot in fps system and metre in mks system. The official international system of units is the SI system (Systeme Internationale d'Units) and commonly employed in engineering and science. The basic units in SI system are given in Table 1-1. Primary units are the basis for obtaining derived units.

Secondary units or *derived units* are those that are made by the inclusion of primary units.

For example, acceleration is a secondary unit. It is expressed as length/time^{-2}. Other examples of derived units in SI units are given in Table 1-2. For these units, alternative base units are given in B part of Appendix II.

TABLE 1-1
Basic Units in SI System

Measurement/Quantity	*Unit*	*Symbol*
Length (L)	Metre	m
Mass (m)	Kilogram	kg
Time (t)	Second	s or sec
Amount of substance	Mole	mol
Temperature	Kelvin	K
Electric current	Ampere	A
Luminous intensity	Candela	cd

All physical quantities consist of two parts.

1. **Unit** : It indicates about the quantity and gives the standard by which it is measured (examples are centimetre, foot, second, pound, grams).
2. **Number** : It denotes the number of units needed (examples are one, two, three etc.).

These two parts together they make a physical quantity. It is essential to specify both the parts, whenever a physical quantity is expressed in the engineering.

Supplementary units : Two supplementary units are at present defined, the radian and the steradian, which are the units of plane and solid angles, respectively.

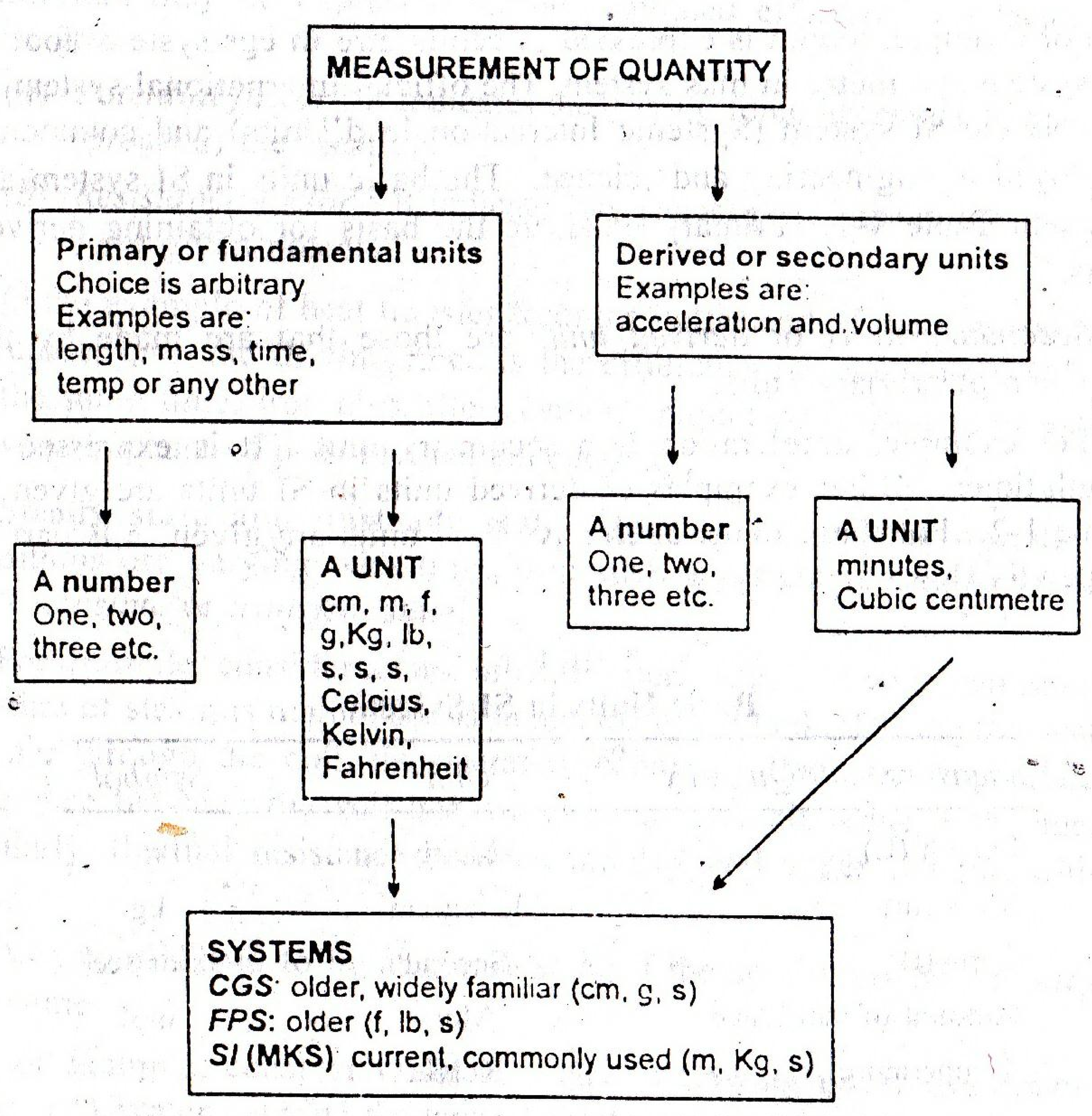


Figure 1-2. Unit systems and relevant ways of expressing a quantity.

Applications : It is essential to be conversant with all the systems and also their inter-conversions. In pharmaceutical engineering, it is necessary to handle a large number of physicochemical data, while selecting the right kind of materials for a process. Most of the literature data are available in the older systems such as cgs and fps systems. Therefore, it is necessary to be expert in all the systems of units.

TABLE 1-2
Some Derived Units in SI System

Measurement/ Quantity	*Unit*	*Symbol*
Force	newton	N
Energy	joule	J
Power	watt	W
Pressure	pascal	Pa
Frequency	hertz	Hz
Electric charge	coulomb	C
Electrical potential	volt	V
Electrical resistance	ohm	Ω

Inter Conversions

Any quantity can be converted from one system to other by the use of conversion factors.

Conversion factor is a pure number and simply the ratio of the magnitude of the unit in one system to that of the corresponding unit in the other system.

Conversion factors are simply multiplication factors. For example, the length expressed in fps system is 10 feet. To convert it from fps to SI system, the conversion factor is 0.3048, i.e., 1 foot = 0.3048 metre.

$$\text{Hence, } 10 \text{ feet} \times 0.3048 \times 10 = 3.048 \text{ metre}$$

It is always better to make a mental-picture of a unit, which will give a large figure (i.e., number). Then the conversion factor should be applied as direct proportionality or inverse proportionality. This can be illustrated here.

In the above example, the conversion factor is 0.3048. Metre (mks system) has higher magnitude compared to feet (fps system). Therefore, metre has a small number compared to the corresponding number in feet. Hence, foot has to be multiplied by the conversion factor to get metre.

$$10 \text{ feet} = 10 \times \text{conversion factor} = 10 \times 0.3048 = 3.048 \text{ metre}$$

Conversely, metre should be divided by conversion factor to obtain feet. For example,

$$3.048 \text{ metre} = \frac{1}{0.3048} \times 3.048 = 10 \text{ feet.}$$

Inter-conversion between SI system and cgs system is simple, because both use same standards for time and temperature. Mass can be converted from one system to the other. Some conversion factors for primary and secondary units between different systems are in tables 1 and 2 of Appendix III.

Temperature is normally denoted in degrees by Celsius (°C), or Fahrenheit (°F) or Kelvin (K) scale. The thermodynamic temperature scale is called the Rankine scale, in which the temperature is denoted by degrees Rankine. Their relationships are given in Table 3 of Appendix III.

Practice Problem 1-1. The unit of viscosity in the cgs system is the poise, which is equal to 1 dy.s/cm². If the fluid has a viscosity of 0.20 poise, calculate the corresponding value in SI units (Pa·s).

Solution: Data - The units are:

$$\text{Poise} = \frac{\text{dy.s}}{\text{cm}^2} = \frac{\text{g}}{\text{cm·s}}$$

The viscosity in SI units and its conversion into base units may be written as:

$$\text{Viscosity} = \text{Pa·s} = \frac{\text{N·s}}{\text{m}^2} = \frac{\text{kg·m·s}}{\text{s}^2\text{·m}^2} = \frac{\text{kg}}{\text{s·m}}$$

The conversion factor can be determined as follows. From the conversion Table of Appendix III, the following factors are obtained.

$$1 \text{ g} = (1/1000) \text{ kg}; \ 1 \text{ cm} = (1/100) \text{ m};$$

By substituting the above terms for units

$$\frac{\text{g}}{\text{cm.s}} = \frac{(1/1000) \text{ kg}}{\text{s} \times (1/100) \text{ m}} = \frac{100 \text{ kg}}{1000 \text{ m} \times \text{s}} = \frac{1 \text{ kg}}{10 \text{ m.s}} = 0.1 \text{ kg/m·s}$$

$$0.20 \text{ poise} = 0.2 \times 0.1 \text{ Pa·s} = 0.02 \text{ Pa·s}$$

Practice Problem 1-2. The density of talc is reported as 2.7 g/ml. Express the same in SI system (kg/m³).

Solution: The given unit of density is g/ml is to be converted to kg/m³. g/ml is also equal to g/cm³. From the conversion Table 1 of Appendix III, the following factors are obtained.

$$1 \text{ g} = (1/1000) \text{ kg}; \ 1 \text{ cm}^3 = (1/100) \text{ m}^3.$$

The conversion factor may be obtained as follows.

$$\frac{\text{g}}{\text{cm}^3} = \frac{(1/1000) \text{ kg}}{(1/100)^3 \text{ m}^3} = \frac{1000000 \text{ kg}}{1000 \text{ m}^3} = \frac{1000 \text{ kg}}{\text{m}^3} = 1000 \text{ kg/m}^3$$

The conversion factor = 1000

$$2.70 \text{ g/ml} = 1000 \times 2.7 \text{ kg/m}^3 = 2700 \text{ kg/m}^3.$$

Practice Problem 1-3. In the literature, mass transfer coefficients in the gas phase are often reported in terms of lb·mol/h·ft²·atm. Determine the conversion factor by which the above must be multiplied in order to obtain the corresponding value of kg·mol/s·m²·Pa.

Solution: The given units $\frac{\text{lb·mol}}{\text{h·ft}^2\text{·atm.}}$ units into which converted $\frac{\text{kg·mol}}{\text{s·m}^2\text{·Pa}}$

From conversion Table 1 of Appendix III, the following conversion factors can be obtained.

$$\text{lb} = 0.4536 \text{ kg}; \ \text{ft}^2 = 0.093 \text{ m}^2; \ \text{h} = 60 \times 60 \text{ s}; \ \text{atm.} = 1.01325\times10^5 \text{ Pa}$$

Substituting the values in the equation gives:

$$\frac{\text{lb·mol}}{\text{h·ft}^2\text{·atm.}} = \frac{0.4536 \text{ kg·mol}}{0.093 \text{ m}^2 \times 60 \times 60 \text{ s} \times 1.01325 \times 10^5 \text{ Pa}}$$

$$= \frac{0.4536 \text{ kg·mol}}{0.093 \times 3600 \times 1.01325 \times 10^5 \text{ m}^2\text{·s·Pa}} = \frac{0.4536 \text{ kg·mol.}}{339.236 \times 10^5 \text{ m}^2\text{·s·Pa}}$$

$$= 1.337 \times 10^8 \text{ kg/m}^2\text{·h·Pa.}$$

The conversion factor for lb/ft²·h·atm. = 1.337 x 10⁸ kg/m²·h·Pa.

Practice Problem 1-4. The overall coefficient of heat transfer is 200 Btu/h·ft²·F. Convert the same into SI units [W/m².K].

Solution:

The given units of $\frac{\text{Btu}}{\text{h.ft}^2\text{·F}}$ into units of $\frac{\text{W}}{\text{m}^2\text{·K}}$

The Btu's equivalent in SI units is J/s, while J/s is equal to W. Therefore, J/s is considered in place of W for obtaining conversion factor.

$$\frac{\text{Btu}}{\text{h·ft}^2\text{.°F}} \text{ to } \frac{\text{J}}{\text{s·m}^2\text{·K}}$$

From the conversion tables 1 & 3 of Appendix III, the following relationships can be obtained.

$$1 \text{ Btu} = 1.0551\times10^3 \text{ J}; \ 1 \text{ h} = 60 \times 60 \text{ s}; \ 1 \text{ ft}^2 = 9.290\times10^{-2} \text{ m}^2; \ 1°\text{F} = (1/1.8) \text{ K}$$

Substituting the above conversion factors into the above equation gives:

$$\frac{\text{Btu}}{\text{h.ft}^2\cdot{}^\circ\text{F}} = \frac{1.0551 \times 10^3 \text{ J}}{60 \times 60 \times 9.290 \times 10^{-2}.1/1.8 \text{ s}\cdot\text{m}^2\cdot\text{K}}$$

$$= \frac{1.0551 \times 10^3 \text{ J} \times 1.8}{3600 \times 9.290 \times 10^{-2} \text{ s}\cdot\text{m}^2\cdot\text{K}} = \frac{1899.18 \text{ J}}{334.44 \text{ s}\cdot\text{m}^2\cdot\text{K}}$$

$= 5.6787$ J/s·m²·K

Since J/s = W, it can be included in the above expression to get units 5.6787 W/m²·K. Therefore, the conversion factor = 5.6787.

200 Btu/h·ft²·°F = 200 × 5.6787 W/m²·K = 1135.74 W/m²·K

DIMENSIONS–FORMULAE, EQUATIONS AND ANALYSIS

Dimensional Formulae

A dimensional formula is a formula that explains the way in which fundamental units enter into the operation.

Dimensional formula expresses the quantity in secondary units. For example, the dimensional formula for acceleration is:

$$[a] = l \cdot t^{-2} \qquad (6)$$
$$= \text{length} \times \text{time}^{-2}$$

Equation (6) can be explained as follows. Acceleration is defined as velocity per unit time.

$$[a] = \frac{\text{velocity}}{\text{time}} \qquad (7)$$

Velocity is defined as a distance per unit time. Therefore, acceleration can be written as:

$$[a] = \frac{\text{Distance (length)}}{\text{time} \times \text{time}} = l \cdot t^{-2} \qquad (8)$$

The symbol $[a]$ means the dimensional formula of the quantity of 'a'.

Applications : Dimensional formulae are used in order to convert the secondary units of one system into another. In these calculations, conversion factors are used cautiously. Then, the physical quantity is obtained in another system.

The dimensionless equations are derived from basic laws mathematically, no matter however complicated they may be. An equation in which all terms have same dimensions is known as *dimensionally homogeneous equation*.

For example, consider equation for Reynolds number.

$$Re = \frac{Du\rho}{\eta} \qquad (9)$$

where D = diameter of the pipe, m
u = velocity of flow, m/s
ρ = density of the fluid, kg/m³
η = viscosity of the fluid, Pa·s

Consider the units in the numerator in equation (9)

$$Du\rho = \text{m} \times \frac{\text{m}}{\text{s}} \times \frac{\text{kg}}{\text{m}^3} = \frac{\text{kg}}{\text{s}\cdot\text{m}}$$

Consider the units in the denominator in equation (9).

$$\eta = \text{Pa}\cdot\text{s} \qquad (10)$$

Since, Pa = kg/m·s², it can be substituted in equation (10)

$$\eta = \frac{\text{kg} \times \text{s}}{\text{m} \times \text{s}^2} = \frac{\text{kg}}{\text{m}\cdot\text{s}}$$

Therefore, equation (9) may be written as:

$$\text{Re} = \frac{\text{kg/m}\cdot\text{s}}{\text{kg/m}\cdot\text{s}} = \text{dimensionless number}$$

Hence equation (9) is considered as dimensionless equation.

Consider another equation as a variation. For example, falling of a body in time, t, can be expressed as:

$$S = ut + (^1/_2)gt^2 \qquad (11)$$

where S = vertical distance, length
u = initial velocity, distance/time
t = time
g = acceleration due to gravity, distance/time²

In equation (11), first and second terms are expressed separately as follows:

$$ut = \text{velocity} \times \text{time} = \frac{\text{distance (length)}}{\text{time}} \times \text{time} = \text{distance (length)}$$

$$\frac{1}{2}gt^2 = \frac{\text{distance (length)}}{\text{time}^2} \times \text{time}^2 = \text{distance (length)}$$

Each term has the units of length. Equation (11) can be made dimensionless by dividing by 'S'.

$$1 = \frac{ut}{S} + \frac{1}{2} \cdot \frac{gt^2}{S} \quad (12)$$

In equation (12), the dimensions get cancelled and each term is dimensionless.

The **advantages** of dimensionless equations are:

1. Unit of any system (cgs or fps or SI) can be used without introducing conversion factors. For example, length in either metres or feet can be substituted in equation (11).
2. Dimentionless equations are based on theoretical principles. They contain variables affecting the physical process.

Dimensional Equations

Dimensional equation is defined as an equation, which contains terms of varying dimensions as it is obtained by empirical methods.

Experimental results are correlated by empirical means. Therefore, dimensional consistency is ignored. Such equations are also known as *dimensionally non-homogeneous equations.*

For example, the rate of heat loss (by conduction and convection) from a horizontal pipe to the atmosphere may be written as:

$$\frac{q_c}{A} = 0.5 \frac{(\Delta t_s)^{1.25}}{(D'_o)^{0.25}} \quad (13)$$

where q_c = loss of heat, Btu/h
A = pipe surface, ft^2
Δt_s = excess of temperature of the pipe wall over that of atmosphere, °F
D'_o = diameter of the pipe, in

The quantities substituted for the terms must be expressed in the units mentioned above. For example, D'_o may be substituted only in inches, not in feet. The reasons are that the numerical coefficients such as 0.5, 1.25 and 0.25 are applicable for those units.

The **disadvantage** of this equation is that it has limited applications. It is particularly used for calculations of a system under specified conditions.

Dimensional Analysis

In the pharmaceutical engineering, many physical problems have been solved completely by theoretical and mathematical methods. On the other hand, there are still many situations wherein empirical relationships have been established over a period of time; since theoretical relationships have failed to satisfy experimental results. Common examples related to these problems are - fluid flow, heat flow and mass transfer.

Dimensional analysis is an important tool to convert the empirical relationships into theoretical principles on a rational basis.

Dimensional analysis assumes that there must exist a relationship among all the factors affecting a process. This technique involves the following steps.

(1) All the factors are to be identified, which are important in the problem. Initial stages, empirical relationship may be adequate.
(2) These factors are grouped together into fewer numbers and expressed as dimensionless groups.
(3) Such groups are entered into final equation.
(4) Such equations are correlated to the possible physical laws.
(5) A possible mathematical solution is obtained.

In the above analysis, the first step is to consider the units for the verification of factors. For example, in the experiments on the fluid flow, the factors involved are listed below.

- pipe diameter (D), m — viscosity (η), Pa·s
- velocity (u), m/s — density (ρ), kg/m^3

These factors are varied as one at a time. Then the results are combined. It is shown by dimensional analysis that these factors must appear in a dimensionless group as shown below.

$$\frac{Du\rho}{\eta} \text{ or } \text{m}\,\frac{\text{m}}{\text{s}} \cdot \frac{\text{kg}}{\text{m}^3} \cdot \frac{1}{\text{Pa·s}} = \frac{\text{kg}}{\text{s·m·Pa}} = \frac{\text{m·s}^2\text{·kg}}{\text{m·s}^2\text{·kg}}$$

This equation is expressed as Reynolds number, which has no dimensions. This example illustrates the success of the dimensional analysis. But heat transfer experiments on fluids involve about 11 factors. A total of five different expressions are obtained. Still dimensional analysis could provide a satisfactory equation to describe the heat transfer process.

Advantages : (1) Dimensional analysis reduces drastically the number of independent variables that effect the problem.

(2) This analysis does not yield numerical values in the equation.

(3) This helps in constructing dimensionless (dimensionally homogeneous) equation.

(4) Very useful for any system of units (cgs or fps or SI).

Disadvantages : Dimensional analysis is a difficult process, if enough knowledge is not available about the physics of the situation.

STOICHIOMETRIC EQUATIONS—BALANCING

Stoichiometry means carrying out of calculations based on quantitative relationships.

The numerical problems involving the use of stoichiometric equations are known as *stoichiometric calculations.*

A chemical reaction is a symbolic representation of a chemical change. Each chemical reaction is expressed in the form of an equation. This is obtained by balancing the atoms of each of the species involved in the reaction. The initial constituents that take part in the reaction are called the *reactants*, and the final constituents that are formed by the reaction are called the *products*. For example, hydrogen and oxygen react to form water. This reaction is expressed as:

Skeleton equation: $H_2 + O_2 \longrightarrow H_20$ (14)

In equation (14), two hydrogen atoms are present on each side. On the left side, two oxygen atoms are present and on right side one oxygen atom is present. Moles can be multiplied or divided by smallest possible integer to obtain a balanced equation. Hence, equation (14) may be balanced as:

$$H_2 + (^1/_2)O_2 \longrightarrow H_20 \quad (15)$$

Balanced equation: $2H_2 + O_2 \longrightarrow 2H_20$ (16)

Equation (16) indicates that one mole of hydrogen and half mole of

oxygen combine to form one mole of water. The reaction may also takes place in reverse direction. The coefficients 2, 1 and 2 in equation (16) are called *stoichiometric coefficients.*

According to the law of conservation of mass, total mass of reactants must be equal to the total mass of products in a reaction. In other words, the number of atoms of each kind in the reactants and products must be the same.

A *balanced chemical equation* indicates the exact number of various elements participating in the reaction.

Balancing is done by inspection. Balanced chemical equations are quantitative expressions of chemical changes. Hence, they enable us to work out the masses of substances reacting together. A few examples are given below.

Applications : (1) Stoichiometric equations (and balancing) helps in understanding the quantitative relationship between different reactants. For example, the ratios 2:1 (equation 16), 1:1 (equation 14) etc.

(2) The amount of reactants to be added for carrying out a reaction can be determined theoretically.

Practice Problem 1-5. Nitrogen combines with hydrogen under suitable conditions to form ammonia. Write the equation and balance it.

Solution: Nitrogen and hydrogen are bi-atomic molecules. The formula of ammonia is NH_3. The reactants and products can be written as:

Skeleton equation: $N_2 + H_2 \longrightarrow NH_3$ (i)

Nitrogen atoms on both sides of equation (i) can be balanced by multiplying NH_3 by 2. In the next step, hydrogen atoms can be made equal both sides by multiplying H_2 by 3. Now, the balanced equation becomes:

Balanced equation: $N_2 + 3H_2 \longrightarrow 2NH_3$ (ii)

Practice Problem 1-6. Carbon combines with oxygen to give carbon dioxide. Write chemical equation and balance it.

Solution: Carbon normally exists in mono-atomic state (C). Oxygen exists as diatomic (H_2). Carbon dioxide is represented by CO_2. Then the skeleton equation may be written as:

Skeleton equation: $C + O_2 \longrightarrow CO_2$ (i)

The number of elements present on the left-hand side of equation (i) is equal to the right-hand side of the equation. Therefore, balanced equation is same as the skeleton equation.

Practice Problem 1-7. Write the balanced equation for the combustion of ethane.

Solution: Combustion means complete oxidation of a substance in the presence of air (oxygen). The products of combustion are normally carbon dioxide and water. Therefore, the equation of the combustion of ethane may be written as:

Skeleton equation: $C_2H_6 + O_2 \longrightarrow H_2O + CO_2$ (i)

On the left side of equation (i), the number of carbons is two, while on right hand-side the number of carbon is one. Therefore, multiply CO_2 by 2. Then, equation (i) can be changed with respect to carbons as:

$$C_2H_6 + O_2 \longrightarrow H_2O + 2CO_2 \quad \text{(ii)}$$

On the left hand-side of equation (ii), the number of hydrogen atoms is six, while on the right hand-side, hydrogen atoms are two. Therefore, multiply H_2O by 3. Then equation (ii) changes with respect to hydrogen as:

$$C_2H_6 + O_2 \longrightarrow 3H_2O + 2CO_2 \quad \text{(iii)}$$

On left hand-side of equation (iii), the number of oxygen atoms is two, while on the right hand-side, the oxygen atoms are seven (3 + 4). Therefore, multiply O_2 by 7/2. Then, equation (iii) can be changed with respect to hydrogen as:

$$C_2H_6 + (7/2)O_2 \longrightarrow 3H_2O + 2CO_2 \quad \text{(iv)}$$

The equation (iv) is balanced. But fractions can be removed by multiplying the entire equation by 2. Then, the balanced equation is:

Balanced equation: $2C_2H_6 + 7O_2 \longrightarrow 6H_2O + 4CO_2$ (v)

The above examples illustrated the methods of balancing chemical equations.

Practice Problem 1-8. Calculate the mass of oxygen obtained by the complete decomposition of 5.0 g of potassium chlorate (K = 39.1; Cl = 33.5; O = 16).

Solution: The equation for the given reaction may be written as:

$$KClO_3 \longrightarrow KCl + O_2$$

Balancing of equation can be with respect to the number of moles of oxygen.

$$2KClO_3 \longrightarrow 2KCl + 3O_2$$

In other words, 2 moles of $KClO_3$ yield 3 moles of oxygen.

2[39.1 + 35.5 + 3(16)] g of $KClO_3$ yields 3(2 x 16) g of oxygen

245.2 g of $KClO_3$ yield 96 g of oxygen

5.0 g of $KClO_3$ yield ? g of oxygen

$$\frac{96 \times 5.0}{245.2} = 1.958 \text{ g of oxygen}$$

The mass of oxygen obtained is 1.958 g.

Glossary of Symbols

A = Pipe surface, ft^2
cgs = Centimetre-gram-second.
D = Pipe diameter, m.
η = Viscosity, Pa·s.
F = Driving force.
fps = Foot-pound-second.
g = Acceleration due to gravity, m/s^2.
M = Molecular weight of individual components.
mks = Metre-Kilogram-second.
n = Number of moles.
R = Resistance.
R = Rankine.
ρ = Density, kg/m^3.
S = Vertical distance, m.
SI = Systeme Internationale.
u = Velocity, m/s.
t = Time, s.
W = Weight of individual components.

QUESTION BANK

Each question carries 2 marks

(1) Describe the principle of stoichiometry with a suitable example.
(2) Highlight the importance of unit operations in pharmaceutical engineering
(3) Describe the molecular concept of stoichiometry.
(4) Give an expression to calculate the average molecular weight of a mixture.
(5) How is the rate of a reaction expressed?
(6) Distinguish between steady state and non-steady state.
(7) Distinguish between equilibrium and steady state.
(8) Define the term 'dimensionless equation' with the help of an example.
(9) Define dimensional equation. What are its limitations?
(10) Define the term 'dimensionless equation'. What are its advantages?

Each question carries 5 marks.

(1) Describe 'unit operation' and 'unit process'. Give two examples each.

(2) Explain the term 'unit operation'. Describe the basic principles of various unit operations used in pharmaceutical and other associated industries.

(3) Explain the term 'mass balance' and 'energy balance'. What are its applications?

(4) Give an account of unit systems and their inter-conversions.