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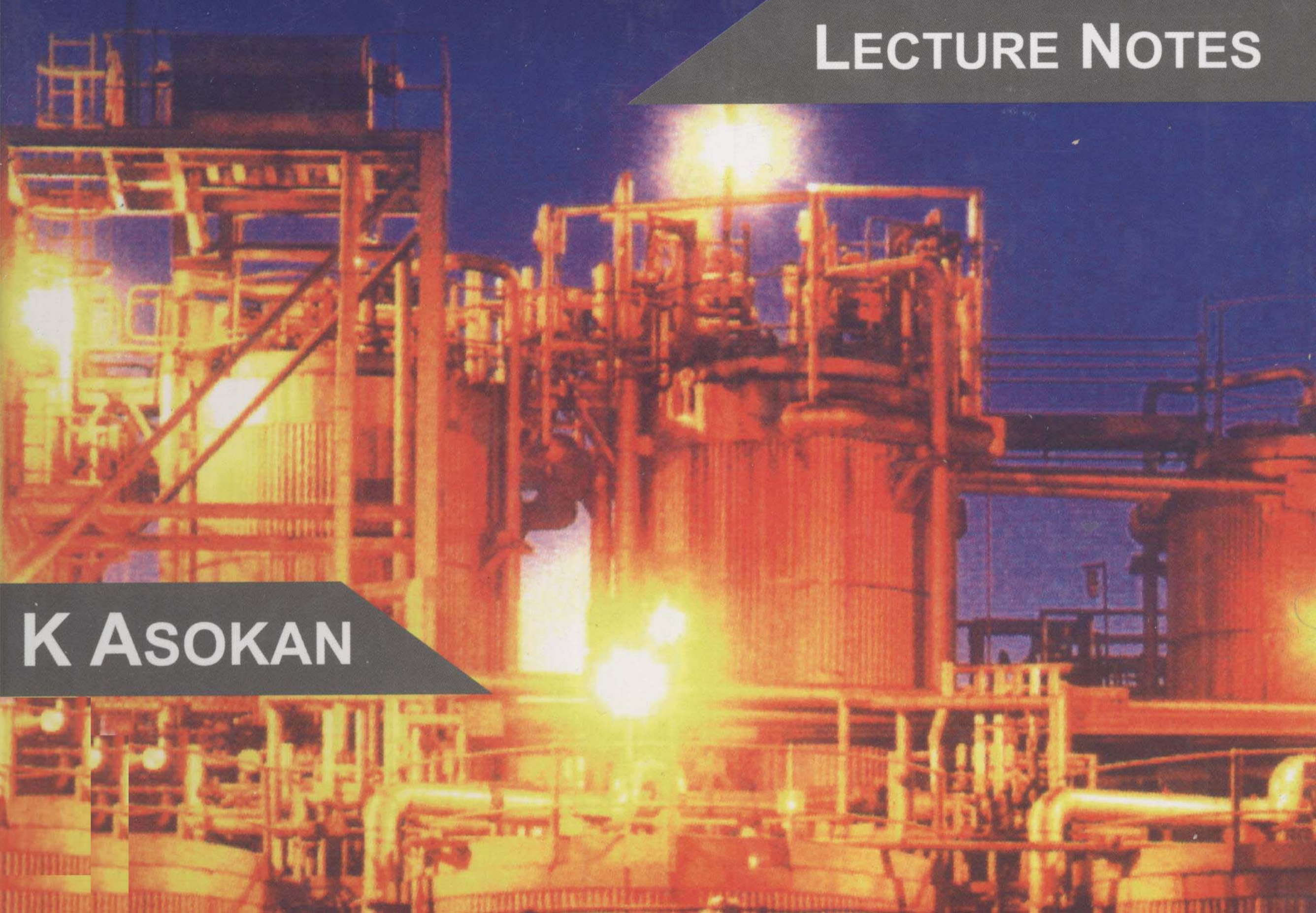
Chemical Process Calculations

LECTURE NOTES



K ASOKAN

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Dedication

This book is dedicated to my dear wife and children. Their comforting presence and willingness to sacrifice their time with me enabled me to concentrate fully on my work.

Preface

Chemical Engineers guide the passage of a product from the laboratory to the market place, from idea or prototype to a functioning article or process, from theory to reality. They design and operate large-scale chemical process equipment and units safely and efficiently, and in an environmentally responsible manner. They produce a diverse range of materials from fuels and fertilisers to processed foods, life-saving pharmaceuticals and filtered clean water. All this requires a thorough understanding of the physical and chemical aspects of materials as well as the energy balance of the processes involved. A chemical engineer can get this knowledge by taking a course on chemical process calculations.

The subject matter of this book is treated in eight chapters divided on conceptual basis. In each chapter, the fundamental principles are explained in simple language, followed by illustrations for clarity. At the end of each chapter, problems have been given for the learner to solve. In all there are 173 worked examples and 154 exercise problems.

The book is intended as a textbook for students taking a diploma in chemical technology, undergraduate chemical engineering and biotechnology, and postgraduate course in applied chemistry.

Karaikudi
July 2007

K Asokan

Acknowledgements

I would like to express my deep sense of gratitude to the following people who have all made this book possible: Professor A K Shukla, Director, Central Electrochemical Research Institute, Karaikudi for his encouragement; my colleague, Dr K Subramanian, for his mental, moral and physical help during the course of preparation of the book, and Mr S Sakthivel, for his neat and patient typing of the material.

Karaikudi
July 2007

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Contents

1 Dimensions, Units and Conversions

Nearly every engineering problem encountered involves dimensions: the *length* of a house, the *mass* of a vessel, the *velocity* of a projectile, the *force* of the air resistance on a motor car, and so on. These *dimensions* can be expressed using specific *units*. For example, length can be expressed in feet, mass as kilograms, velocity as miles per hour, and force as newtons.

The objective of this chapter is to explain the use of dimensions and units in engineering calculations, and to introduce the standard systems of units that are used.

FUNDAMENTAL QUANTITIES AND DERIVED QUANTITIES

Dimensions are used to describe physical quantities. Physical quantities like length, mass, time, electric current, temperature and luminous intensity are called *fundamental quantities*. All other physical quantities like area, volume, velocity, acceleration, force and others, which can be expressed in terms of the fundamental quantities are called *derived quantities*. For example, area is length times length, volume is area times length, velocity is length divided by time, acceleration is velocity divided by time, force is mass times acceleration and so on.

FUNDAMENTAL UNITS AND DERIVED UNITS

The process of determining the number of times a quantity is bigger than a standard quantity is known as measurement. Thus measurement means comparison with a certain standard of the same kind. The accepted standard that is used for comparison of a physical quantity is known as a *unit*. Units in which fundamental quantities are measured are called *fundamental units*. The units of derived physical quantities are expressed in terms of the fundamental units and are called *derived units*.

ENGLISH SYSTEM OF UNITS

The common system of units used in the United States is the English system. In the English system of units, the unit of length is the foot, the unit of mass is the pound mass, and the unit of time is the second. It is also known as the **FPS** system. Units are arbitrary, based on a standard that is developed and agreed upon within a system. Most English system units were inherited from the Romans. For example, the unit of length comes from the average length of a man's foot, and the mile was the average distance a Roman soldier could travel in 1000 paces.

The English system is confusing for several reasons. First, the unit of force is also called the pound, and is defined as one pound mass times the standard acceleration of gravity. It uses non-decimal conversion constants such as 12 inches per foot, 5 280 feet per mile, 43 560 square feet per acre, and 231 cubic inches per gallon.

SI SYSTEM OF UNITS

A more rational, decimal-based system of units was developed in France during the 1700s and was adopted by France in 1795. This system was called the **Metric System**, from the Greek word meaning 'to measure', and has become the standard system in science in much of the world. The standard form is now known as the International System or the **SI system**: The basic unit of length is the metre, the basic unit of mass is the kilogram, and the basic unit of time is the second. The main advantage of this system is that the conversion constants to all other units within the system are decimals. Today there is an international standard for the metre, the kilogram, the second, the ampere of electricity and the candela of light.

SI Base Units

The International System has seven base units from which nearly all the other units are derived.

Table 1.1 SI Base Units

Physical quantity	Name of unit	Symbol
Length	metre	m
Mass	kilogram	kg
Time	second	s
Electric current	ampere	A
Temperature	kelvin	K
Amount of substance	mole	mol
Luminous intensity	candela	Cd

SI Derived Units

The International System has numerous derived units of which many have special names (Table 1.2).

SI Prefixes

In general, numbers should be expressed using appropriate multipliers such that they fall between 0.1 and 1000; 1 250 m is best written as 1.25 km (Table 1.3).

Table 1.2 SI Derived Units

Physical quantity	Name of SI unit	Symbol of SI unit	In SI base units
Force	newton	N	= kg m s^{-2}
Pressure	pascal	Pa	= kg m^{-1} s^{-2}
Energy	joule	J	= kg m^2 s^{-2}
Power	watt	W	= kg m^2 s^{-3}
Charge	coulomb	C	= A s
Frequency	hertz	Hz	= s^{-1}

Table 1.3 SI Prefixes

Multiple	Prefix	Symbol	Multiple	Prefix	Symbol
10^{-1}	deci	d	10	deca	da
10^{-2}	centi	c	10^2	hecto	h
10^{-3}	milli	m	10^3	kilo	k
10^{-6}	micro	μ	10^6	mega	M
10^{-9}	nano	n	10^9	giga	G
10^{-12}	pico	p	10^{12}	tera	T
10^{-15}	femto	f	10^{15}	peta	P

Rules and Conventions in the Use of SI Units

1. The units named after a scientist should not be written with a capital initial letter.
   Example: 10 newtons not 10 Newtons; 5 watts not 5 Watts
2. The symbol for a unit named after a scientist should be written with a capital initial letter.
   Example: 20 N not 20 n
3. The symbol for all other units should not be written with a capital letter.
   Example: m for metre and not M
4. Only the singular form of the unit is to be used.
   Example: 5 kg and not 5 kgs
5. No fullstop or any other punctuation mark should be used within or at the end of the unit.
   Example: 100 m and not 100 m. 50 kg m^{-3} and not 50 kg m^{-3}.
6. When temperature is indicated as kelvin, the degree sign is to be omitted.
   Example: 373 K and not 373°K
7. Space is to be left between the numeral and symbol and between symbols of compound units such as velocity, acceleration, and others.
   Example: 30 s and not 30s; 22 m s^{-1} and not 22 ms^{-1}
8. Use of solidus is to be avoided; when used, not more than one solidus should be employed.
   Example: m s^{-2} or m/s^2 and not m/s/s

9. Units must be written in full or using agreed symbols, but no other abbreviation can be used. Example: Amp is not a valid abbreviation for ampere
10. When numerical values fall outside the range of 0.1 to 1000, the numerals should be separated into groups of three with a space replacing the traditional comma. Example: 5 000 and not 5,000 or 5000; 0.030 456 and not 0.030,456 or 0.030456

CONVERSIONS

In a widely expanding world, familiarity with the various systems of units and an ability to convert from one unit to another are essential. In scientific work, length, mass and time are the three fundamental quantities of interest. In engineering, force is an additional fundamental quantity to be taken into consideration. The unit of force in the FPS system is the poundal. It is the force which will give a mass of one pound, an acceleration of 1 ft s^{-2}. The unit of force in the SI units is newton. It is the force, which will give a mass of one kilogram, an acceleration of 1 m s^{-2}.

It is good to be familiar with the concepts of SI units. Whenever, a problem is encountered with FPS units, they can be converted to SI units they can. From this point of view, the conversion factors acquire importance.

Conversion to SI Units

Basic units

Length:	1 foot	= 0.304 8 m
Mass:	1 pound	= 0.453 6 kg
Force:	1 poundal	= 0.138 N

$$\left(\text{Temperature in °F} - 32) \times \frac{100}{180}\right) + 273 = \text{temperature in kelvin}$$

Freezing point of water, 32°F	= 273 K
Normal boiling point of water, 212°F	= 373 K
1 K	= 1.8°F

Derived units

Area:	1 ft^2	= 0.093 m^2
Volume:	1 ft^3	= 0.028 3 m^3
	1 US gallon	= 3.786 L
Pressure	1 inch Hg	= 3.39 kN m^{-2}

$$\begin{aligned} 1\ \text{psi} &= 6.895\ \text{kN m}^{-2} \\ 1\ \text{atm} &= 101\ 325\ \text{N m}^{-2} \\ &= 101.325\ \text{kN m}^{-2} \\ &= 1.013\ 25\ \text{bar} \\ &= 1.033\ \text{kgf cm}^{-2} \\ &= 760\ \text{Torr} \end{aligned}$$

Energy: $1\ \text{Btu} = 1\ 055\ \text{J}$

Power : $1\ \text{HP} = 748\ \text{W}$

ILLUSTRATIONS

1A The temperature inside an oven is 500°F. Report the temperature in SI units.

$$\text{Temperature in kelvin} = (500 - 32) \times \frac{5}{9} + 273 = 533\ \text{K}$$

1B The specific heat of a metal is 2 Btu $\text{lb}^{-1}\ °\text{F}^{-1}$. Find the value in SI units.

$$\text{The specific heat of the metal} = 2\ \text{Btu} \times \frac{1\ 055\ \text{J}}{\text{Btu}} \times \frac{1}{\text{lb}} \times \frac{\text{lb}}{0.453\ 6\ \text{kg}} \times \frac{1}{°\text{F}} \times \frac{1.8°\text{F}}{1\ \text{K}}$$

$$= 8\ 373\ \text{J kg}^{-1}\ \text{K}^{-1}$$

1C 2.5 US gallons of gasoline weigh 16.69 lb. Find the weight of 2 litres of gasoline in kilograms.

$$\text{Weight of gasoline per litre} = 16.69\ \text{lb} \times \frac{0.453\ 6\ \text{kg}}{\text{lb}} \times \frac{1}{2.5\ \text{gallon}} \times \frac{1\ \text{gallon}}{3.78\ \text{L}}$$

$$= 0.799\ 9\ \text{kg L}^{-1} \approx 0.8\ \text{kg L}^{-1}$$

The weight of 2 litres of gasoline is 1.6 kg.

1D Convert a heat transfer coefficient value of 1000 Btu ft^{-2} h^{-1} $°F^{-1}$ into SI units.

$$1000\,\text{Btu ft}^{-2}\,\text{h}^{-1}\,°\text{F}^{-1} = 1000\,\text{Btu} \times \frac{1\,055\,\text{J}}{\text{Btu}} \times \frac{1}{\text{ft}^2} \times \frac{\text{ft}^2}{0.093\,\text{m}^2} \times \frac{1}{\text{h}} \times \frac{\text{h}}{3\,600\,\text{s}} \times \frac{1}{°\text{F}} \times \frac{1.8°\text{F}}{\text{K}}$$

$$= 5\,672.04\,\text{J m}^{-2}\,\text{K}^{-1}$$

1E The latent heat of vapourisation of saturated steam at 250 psi is 1 201.1 Btu lb^{-1}. Convert the pressure and enthalpy values into SI units.

Pressure $$= 250\,\text{psi} \times \frac{6.895\,\text{kN m}^{-2}}{\text{psi}}$$

$$= 1\,723.75\,\text{kN m}^{-2}$$

Enthalpy $$= 1\,201.1\,\text{Btu} \times \frac{1\,055\,\text{J}}{\text{Btu}} \times \frac{1}{\text{lb}} \times \frac{\text{lb}}{0.453\,6\,\text{kg}}$$

$$= 2\,793.56\,\text{kJ kg}^{-1}$$

Problems for Practice

1.1 Make the following conversions

(i) 142 ft^2 h^{-1} to SI units
(ii) 50 psi to kN m^{-2}
(iii) 100 Btu to kJ
(iv) 1000 W to HP
(v) 1000 lb ft^{-3} to SI units
(vi) 100°F to kelvin

1.2 Air flows through a duct at the rate of 200 lb ft^{-2} h^{-1}. Get the air flow rate in kg m^{-2} s^{-1}.

1.3 The heat transfer coefficient in the case of a drying operation is given by the dimensional equation.

$$h_y = 0.01\frac{G^{0.8}}{D_e^{0.2}}$$

where h_y = heat transfer coefficient in Btu $ft^{-2}\ h^{-1}\ {}^{\circ}F^{-1}$

G = mass velocity in lb $ft^{-2}\ h^{-1}$

D_e = equivalent diameter of the air flow channel in feet

Convert the equation to SI units.

1.4 The mass transfer coefficient for a gas absorption operation is given by $k_{ga} = 0.028\, G_y^{0.7} G_x^{0.25}$ where k_{ga} is the gas phase mass transfer coefficient in mol $ft^{-3}\ h^{-1}\ atm^{-1}$. G_y is the gas rate and G_x is the liquid rate in lb $ft^{-2}\ h^{-1}$ respectively. Transform the expression into SI units.

1.5 Fouling factors for ordinary industrial liquids fall in the range of 300 to 1000 Btu $ft^{-2}\ h^{-1}\ {}^{\circ}F^{-1}$. Give this range in SI units.

2 Basic Concepts

The basic chemical principles required for a clear understanding of material and energy balance will be discussed in this chapter. Matter exists in three different forms: solid, liquid and gas. The simplest mode of expressing the quantity of matter is mass. Solids and liquids can be quantified by weighing them in a balance. The volume of liquids can be measured and if their densities are known, their weight can be determined. A gas occupies the entire volume available and quantification requires a knowledge of temperature and pressure. A common unit used to quantify all the three forms of matter is the *mole*.

Amount of Substance The *mole* is the SI unit of amount of substance. It is defined as the amount of substance that contains as many elementary entities as there are atoms in 0.012 kg of carbon. In other words, one mole contains N elementary entities or basic species, where N is the Avogadro number (6.023×10^{23}).

Volume The *cubic metre* is the SI unit of volume, while *litre* is the common unit of volume. One litre is the volume occupied by one kilogram of air-free water at 277 K, the temperature at which its density is maximum.

$$1 \text{ litre (L)} = 1 \text{ dm}^3 = 1000 \text{ cm}^3$$

$$1 \text{ m}^3 = 1 \text{ kL} = 1000 \text{ L}$$

Force The *newton* is the SI unit of force. One newton is the force which when applied to a body of mass 1 kg gives it an acceleration of 1 m s^{-2}.

Pressure Pressure is defined as force acting on unit area. The SI unit of pressure is N m^{-2} or *pascal* (Pa). The *atmosphere* is the common unit of pressure. Pressure is usually measured with the help of a gauge which denotes the difference in the pressure of the vessel and the local atmospheric pressure. This is known as P_g or gauge pressure. Gauge pressure does not reflect the actual pressure of the vessel. To get the actual or absolute pressure (P), atmospheric pressure has to be added to the gauge pressure.

$$\text{Absolute pressure} = \text{Gauge pressure} + \text{atmospheric pressure}$$

$$P = P_g + \text{atmospheric pressure}$$

1 atmosphere gauge (1 atm g) denotes 2 atmospheres absolute, as the atmospheric pressure has to be added to the gauge pressure, as mentioned above. The atmospheric pressure in different units is given below.

$$\begin{aligned}
1 \text{ atmosphere} &= 101\,325 \text{ N m}^{-2} \\
&= 101\,325 \text{ Pa} \\
&= 101.325 \text{ bar} \\
&= 760 \text{ mm Hg} \\
&= 760 \text{ Torr} \\
&= 76 \text{ cm Hg} \\
&= 10.33 \text{ m } H_2O \\
&= 1.033 \text{ kgf cm}^{-2}
\end{aligned}$$

If no letter follows the pressure unit, absolute pressure has to be presumed. Often, pressure is expressed as pressure head.

$$\text{Pressure head} = \frac{\text{absolute pressure}}{\text{density of the barometric liquid}}$$

The common barometric liquids are mercury and water. One atmosphere pressure is equal to 76 cm mercury column or 1033 cm (10.33 m) water column. To convert the height of a mercury column to that of water column, the height of the mercury column has to be multiplied by the specific gravity of mercury, which is 13.6.

Vacuum refers to sub-atmospheric pressure. It is denoted by Torr or Pa or m bar.

Work and power Work is the product of force acting on a body and the distance travelled by the body under its influence. *Joule* is the SI unit of work. When a force of one newton acts on a body and the body moves through a distance of 1 m, the work done is said to be one joule or 1 J.

Power is the rate of doing work. The *watt* is the SI unit of power. $1 \text{ W} = 1 \text{ J s}^{-1}$

Temperature The unit of temperature in the SI system of units is *kelvin* (K). It is 1/273 of the triple point of water, which is 273 K.

$$\text{The normal freezing point of water} = 32°\text{F} = 0°\text{C} = 273 \text{ K}$$

$$\text{The normal boiling point of water} = 212°\text{F} = 100°\text{C} = 373 \text{ K}$$

A difference of 100 on the Celsius scale = 100 on the Kelvin scale = 180 on the Farenheit scale.

∴ One degree on the Kelvin scale = one degree on the Celsius scale = 1.8 degrees on the Farenheit scale.

$$\text{Temperature in farenheit} = \left(\text{Temperature in kelvin} \times \frac{9}{5}\right) + 32$$

$$\text{Temperature in kelvin} = (\text{Temperature in celsius} + 273)$$

Molecular weight The molecular weight is the weight of one mole of a substance. It is also equal to the weight of all the constituent elements of a compound present in one mole.

Atomic weight The atomic weight is the weight of one mole of an element.

Empirical formula The empirical formula shows the ratio of atoms of each element present in a compound.

Example: CH for benzene.

Molecular formula The molecular formula shows the actual number of atoms of each element present in a compound. It is n times the empirical formula, where n is a whole number.

Example: C_6H_6 for benzene.

Equivalent weight The equivalent weight is the number of parts by weight of a substance which will either react with or release in a reaction 1.008 parts by weight of hydrogen, or 8 parts by weight of oxygen, or 35.46 parts by weight of chlorine or one equivalent of any other substance.

Average molecular weight When a system comprises of more than one substance, then the average molecular weight has to be taken into consideration. It is the algebraic sum of the products of mole fraction and molecular weight of each of the components.

$$m = \Sigma m_i x_i$$

where m is the average molecular weight, m_i is the molecular weight of the i^{th} component; and x_i is the mole fraction of the i^{th} component.

The mole fraction of a component is the ratio of the number of moles of that component (n_i) to the total number of moles (n) in the system.

$$x_i = \frac{n_i}{n}$$

If a system comprises of 1 mol of nitrogen and 3 mol of hydrogen, then the mole fraction of nitrogen is 0.25 and that of hydrogen is 0.75. It may also be noted that the sum of the mole fractions of the components of a system is one: $\Sigma x_i = 1$

Boyle's Law Boyle's law states that at constant temperature, the pressure (P) of a given mass of gas is inversely proportional to its volume (V). At constant temperature, $P \alpha \frac{1}{V}$.

Charles' Law Charles' law states that at constant pressure, the volume (V) of a given mass of gas is directly proportional to its absolute temperature (T). At constant pressure, $V \alpha T$.