Chemical Process Calculations CL204

Module-1

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Units & Dimensions

Dimensions are basic concepts of measurement such as, length, time, mass, temperature, etc.

Units are the means of expressing the dimensions, like

length → feet, centimeters.
time → hour, second, minute, day.
mass → kilogram, gram, pound.
Temperature → centrigrade, kelvin, Rankine.

Two most common system

SI unit → Le Systeme Internationale d'units.
/or SI System of units

AE unit → American Engineering system of units.

Fundamental (or basic) dimensions/ units

which are measured independently and are sufficient to describe essential physical quantity.

length, mass, time, Temperature, molar amount.

Derived dimensions / unit.

Those are developed in terms of the fundamental unit.

Energy, Force, power, density.

SI system

Physical quantity.	name of the Basic unit	Symbol.
length	meter, metre	m
mass	kilogramme/ kilogram	kg
Time	Second	s
Temperature	Kelvin	K
molar amount	mole	mol.

basic unit

Derived unit

Derived units

Energy (E) Joule J = Newton x m = $\frac{\text{Newton} \times m \times m^2}{m^2}$

U = internal energy.

$= kg \times \frac{m}{s^2} \times m$ = Pascal $\times m^3$

$= kg.m^2.s^{-2}$ $= Pa.m^3$

Force (F) Newton $N = kg \times \frac{m^2}{s^2}$ (mass x f)

$= kg.m.s^{-2}$ or $J.m^{-1}$

Power (P) watt $W = kg.m.s^{-3} = \frac{J}{S} = J.s^{-1}$.

Density (ρ) kg/m^3 kilogram per cubic meter $kg.m^{-3}$

velocity (v, u) meter, ersecond $m.s^{-1}$

acceleration meter per second squared $m.s^{-2}$

Pressure (P) Newton per square meter / pascal $N.m^{-2}$ or Pa

Heat capacity (C_P) Joule per kilogram per kelvin $J.kg^{-1}.K^{-1} \rightarrow C_P$ symbolized.

Other important derived units are

mass velocity or mass flux.

$= $ kilogram per meter square per secon

$= kg.m^{-2}.s^{-1}$.

Molar velocity $= mol.m^{-2}.s^{-1}$

mass velocity $= u\rho$.

$= m.s^{-1}.kg.m^{-3}$

$= kg.m^{-2}.s^{-1}$

mass flowrate $= u\rho A$. $A =$ flow area.

$= \frac{m}{s} . \frac{kg}{m^3} . m^2$

$\rho =$ density

$u =$ velocity

$= kg.s^{-1}$

Thermal conductivity, $W.m^{-1}.K^{-1}$ (k).

viscosity, $kg.m^{-1}.s^{-1}$ $(\mu) \rightarrow$ symbol

AE system

Length	foot ,	ft .
mass	pound	lb_m
time	second	s
Temperature	degree Rankine degree Fahrenheit	°R °F
molar amount	pound mole	lb mol.

derived unit

Force (F)	pound (Force)	lb_F .
Energy (E	British thermal unit Foot pound (Force)	BTU or $(ft)(lb_F)$
Power	horse power	hp
density	pound per cubic foot	$lb \cdot ft^{-3}$ / lb/ft^3
Acceleration	Feet per second squared	$ft \cdot s^{-2}$

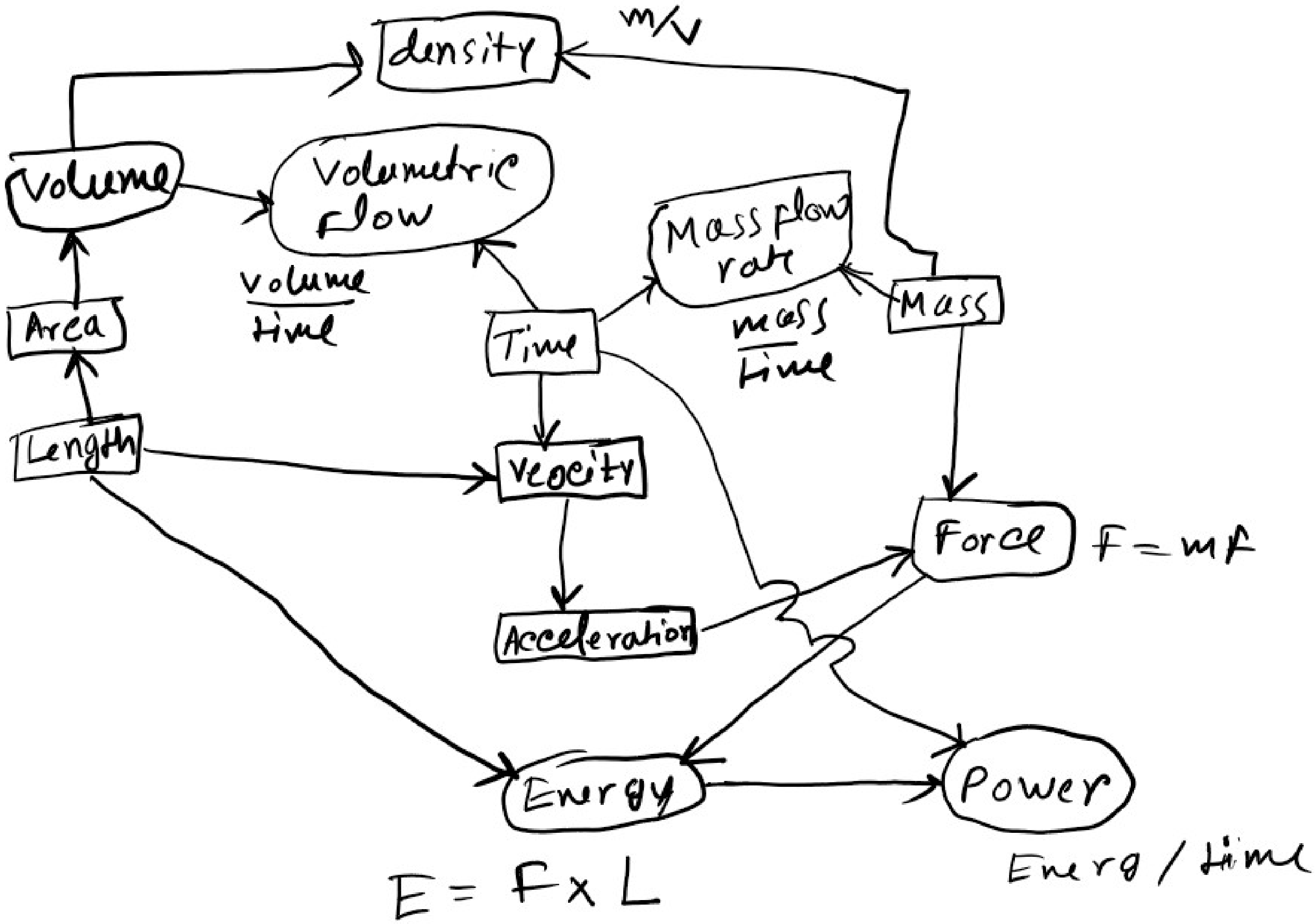
Pressure Pound force per square inch $lb_f \cdot in^{-2}$ / psi (gauge pressure), psia (a for absolute).

∴ Absolute pressure = gauge pressure + Atmospheric pressure.

∴ 1 atm = 14.7 psi

$$20 \text{ psi} = 20 + 14.7 \text{ (psia)}$$
$$= 37.7 \text{ psia}$$

Heat capacity BTU per pound per degree F. → $BTU \cdot lb_m^{-1} \cdot {}^{\circ}F^{-1}$


density
m/V
Volume
Volumetric flow
volume/time
Mass flow rate
mass/time
Area
Time
Mass
Length
Veocity
Force
F = ma
Acceleration
Energy
Power
Energ / time
E = F x L

SI Prefix

Factor	Prefix	symbol.
10^9	giga	G
10^6	mega	M
10^3	kilo	k
10^2	hecto	h
10^1	deka	da
10^{-1}	deci	d
10^{-2}	centi	c
10^{-3}	mili	m
10^{-6}	micro	μ (micron).
10^{-9}	nano	n.

$1\ GJ = 10^9\ J$

$\rightarrow 1\ MJ = 10^6\ J.$

$\boxed{0.09 \text{ poise} = 9\ c.P}$

$1\ c.P = 10^{-2}$ poise

1 poise $= 1\ gm.cm^{-1}.s^{-1}.$

↳ viscosity.

$1\ P = 1\ kg.m^{-1}.s^{-1}$

P = Poiseuille [SI]

Conversion of units.

velocity ft/s → mi/min → m/s.

100 ft/s → mi./hr.

$$100 \frac{\cancel{ft}}{\cancel{s}} \left| \frac{1\ mi}{5280\ \cancel{ft}} \right| \frac{60\ \cancel{s}}{1\ \cancel{min}} \left| \frac{60\ \cancel{min}}{1\ hr} \right.$$

$\downarrow$ mi/s $\downarrow$ mi/min mi/hr

$$= \frac{100 \times 60 \times 60}{5280}\ mi/hr = 68.182\ mi/hr$$

100 ft/s = 68.182 mi/hr.

$$100 \frac{ft}{s} \left| \frac{1\ m}{3.28\ ft} \right. = \frac{100}{3.28}\ m/s.$$

$\searrow$ m/s $= \underline{30.48}$ m/s.

Conversion of cm to in.

$$100\,cm = 100\,\cancel{cm} \,\Big|\, \frac{1\,in.}{2.54\,\cancel{cm}}$$

$$= 39.37\ inch.$$

Conversion of $10\ in^3/day$ & cm^3/min.
volumetric flowrate.

$$10\,\frac{\cancel{in^3}}{\cancel{day}} \,\Big|\, \frac{1\,cm^3}{\left(\frac{1}{2.54}\right)^3 \cancel{in^3}} \,\Big|\, \frac{\frac{1}{24}\,\cancel{day}}{1\,\cancel{hr}} \,\Big|\, \frac{1\,\cancel{hr}}{60\,min}$$

$\to cm^3/day$ $\quad cm^3/hr$ $\quad cm^3/min$

$$= \underline{0.11379}\ cm^3/hr$$

$$= 0.11379 \times (10^{-2})^3\ m^3/hr$$

$$= 0.11379 \times 10^{-6}\ m^3/hr$$

$$= \frac{0.11379 \times 10^{-6}}{60 \times 60}\ m^3/s.$$

Conversion of gravitational accelaration

$$1\ N = 1\ kg \times \frac{m}{s^2} = 1\ kg.m.s^{-2}$$

If a mass of 1 lb_m is hypothetically accelerated at g ft/s^2, where

$$g = 32.2\ ft/s^2$$

SI unit $g = 9.8066 \simeq 9.8\ m/s^2$

$$9.8\ m/s^2 \rightarrow ft/s^2$$

$$9.8\ \frac{\cancel{m}}{s^2}\left|\frac{3.28\ ft}{1\ \cancel{m}}\right.$$

$$= \underline{32.174}\ ft/s^2 \simeq 32.2\ ft/s^2$$

$\Rightarrow F = 1\ lb_f \rightarrow$ where $1\ lb_m$ is accelarated in gravity.

$$1\ lb_f = \frac{1\ lb_m}{}\left|\frac{g\ ft}{s^2}\right|\frac{1\ lb_f\ s^2}{32.174\ (lb_m)(ft)}.$$

$$= 1\ lb_m \times \frac{g}{g_c}.$$

$$g_c = 32.174\ \frac{(ft)(lb_m)}{lb_f\ s^2}$$

g_c is useful in AE system where to convert lb_m to lb_f

Now take

$m = 10\ lb_m$, $h = 10\ ft$.

Potential energy $= mgh$.

$$P = \frac{10\ lb_m}{} \left| \frac{32.2\ ft}{s^2} \right| \frac{10\ ft}{} \left| \frac{(s^2)(lb_F)}{32.174\ (ft)(lb_m)} \right.$$

$$= 100\ (ft)\ (lb_F).$$ Length Force φ AE

SI $m = 10\ lb_m = 10 \times 0.4535\ kg$

$$P = 10 \times 0.4535\ kg \times 9.8\ \frac{m}{s^2} \times \frac{10 \times}{3.28}\ m$$

$$= 980 \times 0.4535\ kg \cdot m^2 \cdot s^{-2}$$

$$= 980 \times 0.4535\ J$$

kinetic energy $= \frac{1}{2} m v^2$ J

Viscosity (μ) · $kg \cdot m^{-1} \cdot s^{-1}$ or $lb_f \cdot hr \cdot ft^{-2}$ or $lb_f \cdot ft^{-2} \cdot hr$

convert 10 $kg \cdot m^{-1} \cdot s^{-1}$ (SI unit) to

AE unit → $lb_f \cdot hr \cdot ft^{-2}$

$$\frac{10\ \cancel{kg}}{\cancel{m} \cdot s} \left| \frac{1000\ \cancel{gm}}{1\ \cancel{kg}} \right| \frac{0.0022\ lbm}{1\ \cancel{gm}} \left| \frac{\cancel{m}}{3.28084\ ft} \right.$$

$$= \frac{10 \times 1000 \times 0.0022}{3.28084}\ lbm \cdot s^{-1} \cdot ft^{-1}$$

$$= 6.70559\ \boxed{lbm \cdot ft^{-1} \cdot s^{-1}} \rightarrow (\mu)$$

(another unit of viscosity).

∴ Now

$$1\ lbm = \frac{1}{32.174}\ lb_f\ s^2 \cdot ft^{-1}.$$

because $\left[\ 1\ lb_f = 32.174\ lbm \cdot ft \cdot s^{-2}\ \right]$

$6.70559\ lbm \cdot ft^{-1} s^{-1}$

$$= \frac{6.70559}{32.174}\ lb_f\ s^2 \cdot ft^{-1} \cdot ft^{-1} \cdot s^{-1}$$

$$= 0.2084\ lb_f \cdot s \cdot ft^{-2}$$

$$= \frac{0.2084}{3600}\ lb_f \cdot hr \cdot ft^{-2}.$$

$$= \underline{0.00005789\ lb_f \cdot hr \cdot ft^{-2}}$$

Thermal conductivity (K) $W \cdot m^{-1} \cdot {}^\circ C^{-1}$
$\rightarrow J \cdot m^{-1} \cdot s^{-2}$] $\rightarrow$ SI

$BTU \cdot hr^{-1} \cdot ft^{-1} \cdot {}^\circ F^{-1}$ [1 BTU = 1055.056 J
= 252.167 cal]

convert $BTU \cdot hr^{-1} \cdot ft^{-1} \cdot {}^\circ F^{-1}$
to $W \cdot m^{-1} \cdot {}^\circ C^{-1}$.

$$1 \frac{\cancel{BTU}}{\cancel{hr} \cdot \cancel{ft} \cdot \cancel{{}^\circ F}} \left| \frac{1055.056\ J}{1\ \cancel{BTU}} \right| \frac{1\ \cancel{hr}}{3600\ s} \left| \frac{3.28\ \cancel{ft}}{1\ m} \right| \frac{\cancel{{}^\circ F}}{\frac{9}{5}\ {}^\circ C}$$

$$= \frac{1 \times 1055.056 \times 3.28 \times 5}{3600 \times 9} \ \frac{J}{s} \cdot m^{-1} \cdot {}^\circ C^{-1}$$

$$= 0.534 \ W \cdot m^{-1} \cdot {}^\circ C^{-1}.$$

$\therefore$ Now $1 \ W \cdot m^{-1} \cdot {}^\circ C^{-1} = 1 \ W \cdot m^{-1} \cdot K^{-1}$.

$\therefore \ 1^\circ C = 1 + 273.15 \ K$

$\therefore \ C_1 \ {}^\circ C = K_1 - 273.15 \ K$

$\therefore \ C_2 \ {}^\circ C = K_2 - 273.15 \ K$

$\therefore \ (C_1 - C_2) \ {}^\circ C = (K_1 - K_2) \ K$.

$\Delta T \ {}^\circ C = \Delta T \ K$

$\therefore$ units in C_p, K, h are in ~~of~~ the form of ΔT. $C_p (1 \ J \cdot kg^{-1} \cdot {}^\circ C^{-1}) = C_p (1 \ J \cdot kg^{-1} \cdot K^{-1})$

$\therefore$ Total heat = $\underline{m \ C_p \ \Delta T}$

Other units are

heat transfer coefficient h.

$\therefore$ h (watt. m^{-2}. K^{-1} / watt. m^{-2}. $°C^{-1}$)

h (BTU. hr^{-1}. ft^{-2}. °F).

Problem

velocity of a fluid measured with a pitot tube is given by,

$$v = \sqrt{\frac{2\Delta P}{\rho}}$$

v = velocity.

ΔP = pressure drop = 15 mm Hg

ρ = density of fluid = 1.20 gm/cm³

Find velocity.

$$\frac{2 \times \Delta P}{\rho} = \frac{2 \times 15\ \cancel{mmHg}}{} \left| \frac{1.01325 \times 10^5 Pa}{760\ \cancel{mmHg}} \right| \frac{cm^3}{1.20\ gm} \left| \frac{(0.01)^3 m^3}{cm^3} \right| \frac{1000\ gm}{1\ kg}$$

$$= \frac{2 \times 15 \times 1.01325 \times 10^5 \times 10^{-6} \times 10^3}{760 \times 1.20} \frac{m^2}{s^2}$$

$$= 3.333\ \frac{m^2}{s^2}$$

$$\therefore \sqrt{\frac{2\Delta P}{\rho}} = \sqrt{3.333}\ m/s = \underline{1.825\ m/s}$$

$$\sqrt{N/m^2 \times \frac{1}{kg \cdot m^{-3}}} = \sqrt{\cancel{kg} \frac{m}{s^2} \frac{1}{m^2} \frac{m^3}{\cancel{kg}}} = m/s$$

$$= m/s$$

Dimensional consistency

Equations must be dimensionally consistent.

$$A_1 \pm A_2 \pm A_3 = A_4$$

Then units / dimensions of terms.

A_1, A_2, A_3, and A_4 will be same.

Each term in an equation as the same net dimensions / units as every other term to which it is added, substracted, or equated.

$\Rightarrow 1\,m \pm 1\,gm \neq$

$\Rightarrow 1\,kg/s \pm 2\,watt \neq$

$1\,m + 3\,m = 4\,m$ ✓

$2\,J + 5\,J = 7\,J$ ✓

$\therefore A_1 \times A_2$ or $A_1 \div A_2$.

A_1 and A_2 units/dimentions must not be same.

They can be different in multiplication or division.

$\Rightarrow$ Mass flux = velocity × density

$= v\rho$

$= m/s \times kg/m^3$

$\Rightarrow kg.m^{-2}.s^{-1}$

Power = $\frac{\text{Energy}}{\text{time}} = \frac{J}{s} =$ watt.

5 watt + 40000 J

$t = 500s$.

5 watt + $\frac{4000\cancel{0}}{5\cancel{00}}\frac{J}{s}$

$5W + 80W = \underline{\underline{85W}}$

van der Walls equation

$$\left(P + \frac{a}{v^2}\right)(v \div b) = RT$$

$P =$ pressure N/m^2

$v =$ m^3/mol.

$\therefore$ a, b are vander Wall constant.

$\Rightarrow$ unit of v and b are same.

b (m^3/mol).

$$\therefore \frac{a}{v^2} = P$$

$$\Rightarrow a = P \times v^2$$

$$= \frac{N}{m^2} \times \left(\frac{m^3}{mol}\right)^2$$

$$= N \cdot m^4 \cdot mol^{-2}$$

$$= \underline{\underline{J \cdot m^3 \cdot mol^{-2}}}$$

$\therefore T = K$

$$\therefore R = \frac{P \times V}{T} = \frac{N}{\cancel{m^2}} \cdot \frac{\cancel{m^3}}{mol \times K}$$

$$= \underline{J \cdot mol^{-1} \cdot K^{-1}}$$

$$R = J \cdot mol^{-1} \cdot K^{-1} \quad \therefore \; {}^{\circ}C = \underline{\underline{K - 273}}$$

$$= \cancel{J \cdot mol^{-1} \cdot ({}^{\circ}C + 273)^{-1}}$$

$$= BTU \cdot lb\,mol^{-1} \cdot {}^{\circ}R^{-1}.$$

$$d = 16.2 - 16.2 \times e^{-0.021t}.$$

$t < 200$.

$d = \mu m$. (μ)

$t =$ second (s).

$$\therefore d = \underline{c_1 - c_2} \, e^{-0.021t}.$$

$0.021 = c_3$

$c_1 = \underline{\underline{\mu m}}$

$c_2 = \mu m$

0.021 or c_3 s^{-1}.

$e^a \cdot e^b \rightarrow$ dimensionless

10^a 10^b.

$\log a$ $\log b$

$$\frac{d}{dx}\sqrt{1+\left(\frac{x}{a}\right)^2} = \frac{2ax}{\sqrt{1+\left(\frac{x}{a}\right)^2}}$$

x = length (m)

a = constant. (m).

$\frac{x}{a}$ = unitless.

$$\frac{m^2}{\text{dimensionless}}$$

The above equation is wrongly expressed

LHS units ≠ RHS units

$$m^{-1} \neq m^2$$

$$C\frac{d}{dx}\sqrt{1+\left(\frac{x}{a}\right)^2} = \frac{2ax}{\sqrt{1+\left(\frac{x}{a}\right)^2}}$$

For correct expression,
the units of C will be m^3

Dimensionless number

Reynolds number; Re or N_{Re}

$$Re = \frac{\text{inertial force}}{\text{viscous force}}$$

$$Re = \frac{D \bar{v} \rho}{\mu}$$

$\bar{v}$ = average velocity of fluid (m/s)
D = diameter of pipe.

For flat plate (flow over a flat plate).

$$Re_x = \frac{x \bar{v} \rho}{\mu}$$

For circular pipe (tube), cross sectional area = $\frac{\pi}{4} D^2$

$$\therefore Re = \frac{\rho \bar{v} \frac{\pi}{4} D^2}{\mu \frac{\pi}{4} D} = \frac{4 \dot{m}}{\pi \mu D}$$

$\dot{m}$ = mass flow rate (kg/s)

Prandtl number, $Pr = \frac{\text{momentum diffusivity}}{\text{Thermal diffusivity}}$

$$= \frac{\mu/\rho}{K/\rho C_p}$$

$$= \frac{\mu C_p}{K}$$

Re (dimension)

$$\frac{\overset{D}{m} \;\Big|\; \overset{\bar{v}}{\frac{m}{s}} \;\Big|\; \overset{\rho}{\frac{kg}{m^3}} \;\Big|\; \overset{\mu}{\frac{m \cdot s}{kg}}}{}$$

= unitless (1).

$$\therefore Pr \text{ (dimensions)}. \frac{\frac{kg}{m \cdot s} \Big| \frac{m^3}{kg}}{W \cdot m^{-1} \cdot K^{-1} \Big| \frac{m^3}{kg} \Big| \frac{kg \cdot K}{J}}$$

$$= \frac{m^2/s}{m^2/s} = \text{unitless (1)}.$$

Nusselt number $Nu = \dfrac{\text{Convective heat transfer}}{\text{conductive heat transfer}}$

$$= \frac{hA\Delta T}{KA\frac{\Delta T}{L}}$$

$$Nu_L = \frac{hL}{k}$$

$\therefore$ L = Length scale (m).

h = heat transfer co-efficient $W/(m^2 \cdot K)$ or $W \cdot m^{-2} \cdot K^{-1}$

k = Thermal conductivity $W \cdot m^{-1} \cdot K^{-1}$.

$$\therefore Nu \text{ (dimensions) } \underbrace{\frac{W}{m^2 \cdot K}}_{h} \Big| \underbrace{\frac{m}{}}_{L} \Big| \underbrace{\frac{m \cdot K}{W}}_{k}$$

$$= \text{unitless } (1).$$

Froude number, $Fr = \dfrac{\text{inertial Force}}{\text{gravity Force}}$

$$= \frac{V^2}{gL} = \frac{m^2}{s^2} \Big| \frac{s^2}{m} \Big| \frac{}{m}$$

$$= (1).$$

Euler number, $Eu = \dfrac{\text{Pressure force}}{\text{inertial forces}}$

$$= \frac{\Delta P}{\rho V^2}$$

$$\therefore \quad Eu \quad \underbrace{\frac{N}{m^2}}_{\Delta P} \Big| \underbrace{\frac{m^3}{kg}}_{\rho} \Big| \underbrace{\frac{s^2}{m^2}}_{V^2} = (1) \text{ dimensionless.}$$

Buckingham Pi Theorem

It states that the functional relationship among q quantities or variables whose units may be given in terms of u fundamental units or dimensions, may be written as $(q-u)$ independent dimensionless groups, called π's.

An incompressible fluid is flowing inside a circular tube of diameter D. The significant variables are pressure drop ΔP, velocity v, diameter D, tube length L, viscosity μ, and density of fluid, ρ.

$\therefore$ Total number of variables $q = 6$

$\therefore$ Fundamental units or dimensions, $u = 3$ (mass, length, time). (M, L, t).

ΔP in $M L^{-1} t^{-2}$

v in $L \cdot t^{-1}$

D in L

L in L.

μ in $M \cdot L^{-1} \cdot t^{-1}$

ρ in $M L^{-3}$.

The number of independent dimensionless group $= q - u = 6 - 3 = 3$.

Thus $\pi_1 = f(\pi_2, \pi_3)$ — (i)

We select a core group of $u = 3$ variables which will appear in each π group and among them contain all the fundamental dimensions.

Now we select D, v and ρ to be core variables common to all three groups.

$\therefore \pi_1 = D^a v^b \rho^c \Delta P$ — (ii)

$\therefore \pi_2 = D^d v^e \rho^f L$ — (iii)

$\therefore \pi_3 = D^g v^h \rho^i \mu$ — (iv)

Now, consider eqn (ii)

$\therefore \; M^0 L^0 t^0 = 1 = L^a \left(\frac{L}{t}\right)^b \left(\frac{M}{L^3}\right)^c \frac{M}{L t^2}$

$\therefore$ component's sum for each fundamental dimension will be zero.

$L: \quad a+b-3c-1=0$

$M: \quad c+1 = 0$

$t: \quad -b-2=0$

$\Rightarrow a=0, \; b=-2, \; c=-1.$

substituting into eqn. (ii)

$$\boxed{\pi_1 = \frac{\Delta P}{v^2 \rho} = N_{Eu}} \quad \text{— (v)}$$

Now consider eqn. (iii)

$$1 = L^d \left(\frac{L}{t}\right)^e \left(\frac{M}{L^3}\right)^f L.$$

$L: \; d+e+1=0$

$M: \; f=0$

$t: \; -e=0$

$\Rightarrow d=-1; \; f=0, \; e=0$

$$\boxed{\therefore \; \pi_2 = \frac{L}{D}} \quad \text{— (vi)}$$

Consider eqn. (iv)

$$1 = L^{g}\left(\frac{L}{t}\right)^{h}\left(\frac{M}{L^3}\right)^{i}\frac{M}{L\cdot t}.$$

L: $g+h-3i-1=0.$

M: $i+1=0.$

t: $-h-1=0.$

$\therefore$ $i=-1,\ h=-1.$ $\Rightarrow g-1+3-1=0$

$\Rightarrow g=-1.$

$$\therefore \pi_3 = \frac{\mu}{Dv\rho} = \frac{1}{N_{Re}}$$

$$\therefore \frac{\Delta P}{v^2\rho} = f\left(\frac{L}{D}, N_{Re}\right).$$

Different forms of density

density $\rho = \frac{m}{V}$ kg/m^3.

Specific volume $\hat{V}$ or $\vartheta = \frac{V}{m}$ m^3/kg

Molar density $= \frac{\rho}{MW}$ mol/m^3.

Molar volume $= \frac{MW}{\rho}$ m^3/mol.

Solution: Homogeneous mixture of two or more components (solid, liquid or gaseous), is called solution.

$V = \sum_{i=1}^{n} V_i$ n = number of components.

$m = \sum_{i=1}^{n} m_i \Rightarrow \rho_{solution} = \frac{m}{V} = \frac{\Sigma m_i}{\Sigma V_i}$

Specific gravity: It is dimensionless ratio.

$$Sp.\ gr\ of\ A = \frac{(g/cm^3)_A}{(g/cm^3)_{ref}} = \frac{(kg/m^3)_A}{(kg/m^3)_{ref}} = \frac{(lb/ft^3)_A}{(lb/ft^3)_{ref}}.$$

∴ The reference substance is water at 4°C.

∴ density of water at 4°C (ref).

$= 1.000\ g/cm^3 = 1000\ kg/m^3 = 62.43\ lb/ft^3$

$\therefore sp.gr = 1.57 = 1.57 \times 1.00\ g/cm^3$

$= 1.57\ g/cm^3$.

$= 1.57 \times 1000\ kg/m^3$.

$= 1570\ kg/m^3$.

$= 1.57 \times 62.43\ lb/ft^3$

$= 97.97\ lb/ft^3$

In the pertroleum industry is in °API scale.

$\therefore$ °API $= \dfrac{141.5}{sp.\ gr.\ \frac{60°F}{60°F}} - 131.5$ (API gravity).

$Sp.\ gr\ \dfrac{60°}{60°} = \dfrac{141.5}{°API + 131.5}$

$\therefore$ 60°F as the standard temperature.

Other specific gravity such as Baume (°Be) and Twaddel (°Tw) exist.

<u>Mole fraction</u>

A, B, C ← mixture or solution.

$$\text{mole fraction of } A = \frac{\text{Moles of } A}{\text{Moles of } (A+B+C)}.$$

$$= \frac{\text{Moles of } A}{\text{Total moles}}.$$

$$\text{Mass fraction of } A = \frac{\text{Mass of } A}{\text{Total mass}}.$$

$$\therefore \text{Mole fraction} = \frac{\text{Mass of } A/M.W_A}{(\text{Mass of } A/M.W_A) + (\text{Mass of } B/M.W_B) + (\text{Mass of } C/M.W_C)}$$

<u>Concentrations</u>

⇒ It refers to the quantity of some substance per unit volume.

* <u>Mass per unit volume</u> ⇒ lb of solute / ft^3 of solution.
g of solute / L of " .
kg " " / m^3 " " .

* <u>Moles per unit volume</u> ⇒ lb mol of solute / ft^3 of solution
g mol of solute / L .
kgmol of solute / m^3.

* Parts per million (ppm) ; Parts per billion (ppb).

⇒ Units of concentrations for extremely dilute solution.

⇒ These are equivalent to mass fraction.

* Molarity (gmol/L) ; molality (mol solute/kg solvent)

normality (equivalents/L solution).
of solute.

Example

SO_2 concentration: 365 $\mu g/m^3$.

particulate matter: 150 $\mu g/m^3$.

CO: 10 mg/m^3

Ozone: 0.12 ppm.

Problem: convert 10.0 ppm HCN in air to mg HCN / kg air.

$$\therefore 10.0 \text{ ppm} = \frac{10.0 \text{ gmol HCN}}{10^6 (\text{air} + \text{HCN}) \text{ gmol}}.$$

Here, HCN in air is extremely low.

$$\therefore 10^6 (\text{air} + \text{HCN}) \text{ gmol} \simeq 10^6 \text{ air gmol}.$$

$$\therefore 10.00 \text{ ppm} = \frac{10.0 \text{ gmol HCN}}{10^6 \text{ gmol air}}.$$

M.W of HCN = 27.03. and air M.W = 29.

$$\therefore 10.00 \text{ ppm} = \frac{10 \text{ gm mol HCN}}{10^6 \text{ gm mol air}} \Bigg| \frac{27.03 \text{ g HCN}}{1 \text{ gmol HCN}} \Bigg| \frac{1 \text{ g mol air}}{29 \text{ g air}} \Bigg| \frac{1000 \text{ mg HCN}}{1 \text{ g HCN}} \Bigg| \frac{1000 \text{ g air}}{1 \text{ kg air}}$$

$$\boxed{= 9.32 \text{ mg HCN/kg air}}$$

For heavier than water.

$$°\text{Baume } (°BE) = 145 - \frac{145}{Sp.gr\ \frac{60°F}{60°F}}$$

For lighter than water

$$°BE = \frac{140}{Sp.gr\ \frac{60°F}{60°F}} - 130$$

$$°\text{Brix} = \frac{400}{Sp.gr.\ \frac{60°F}{60°F}} - 400$$

Concentration

$pH = -\log(H^+)$.

H^+ = H^+ concentration in gm eq/L

7 ph is neutral.

$7 < ph$. is basic $\rightarrow ph > 7$.

$7 < ph$ is acidic $\rightarrow ph < 7$.

For Strong acid.

Weak acid CH_3COOH, hypochlorous acid.

Concentration of $[H^+] = \sqrt{Ma\,Ka}$.

Ka = ionization constant.

Ma = molarity.

Stoichiometry

Stoichiometry provides a quantitive means of relating the amount of products produced by chemical reaction to the amount of reactants.

$$cC + dD \rightleftharpoons aA + bB$$

a, b, c, d are the stoichiometric coefficients for the species A, B, C, and D, respectively.

$$\Rightarrow v_A A + v_B B + v_C C + v_D D = 0 = \sum v_i S_i$$

$v_C = -c$; $v_A = a$

$v_D = -d$; $v_B = b$

reactants to have negative values.

Products to have positive values.

Say $O_2 + 2CO \rightarrow 2CO_2$

$v_{O_2} = -1$; $v_{CO} = -2$; $v_{CO_2} = 2$; $v_{N_2} = 0$.

Balancing Chemical reaction

$$C_6H_{12}O_6 + aO_2 \rightarrow bCO_2 + cH_2O$$

balancing C: $6 = b$; $\Rightarrow b = 6$;

" H: $12 = 2c$; $\Rightarrow c = 6$;

" O: $6 + 2a = 2b + c$.

$\Rightarrow a = 6$;

$\therefore C_6H_{12}O_6 + 6O_2 \rightarrow 6CO_2 + 6H_2O$

Extent of reaction

Extent of reaction $\xi = \frac{n_i - n_{i0}}{\upsilon_i}$

n_i = moles of species i present in the system after the reaction occurs.

n_{i0} = moles of species i present in the system when the reaction starts.

υ_i = coefficient for species i in the chemical reaction

ξ = extent of reaction (moles reacting).
it denotes how much reaction occurs.

20 moles CO + 10 mol O_2 → 15 moles of CO_2.

$2CO + O_2 \rightarrow 2CO_2$

$\upsilon_{CO} = -2,\ \upsilon_{O_2} = -1 \therefore\ \upsilon_{CO_2} = 2.$ $\upsilon_{CO_2} = 2.$

$n_{CO_2} = 15$ mols.

$n_{CO_2,0} = 0$ "

ξ with respect to CO_2 $= \frac{n_{CO_2} - C_{CO_2,0}}{\upsilon_{CO_2}} = \frac{15-0}{2}$

$\boxed{= 7.5}$

∴ 15 moles CO reacted with $\frac{15}{2}$ moles O_2 to produce 15 moles CO_2.

∴ n_{CO} = initial CO − reacted CO.
$= 20 - 15 = 5$ moles.

$n_{CO,0} = 20$.

∴ ξ with respect to CO $= \frac{5-20}{\upsilon_{CO}} = \frac{-15}{-2} = \boxed{7.5}$

. n_{O_2} = initial O_2 − reacted O_2.

$n_{O_2} = 10 - 7.5 = 2.5$

∴ ξ with respect to O_2 $= \frac{2.5-10}{\upsilon_{O_2}} = \frac{-7.5}{-1} = \boxed{7.5}$

Limiting & Excess reaction

The limiting reactant is the species in a chemical reaction that would theoretically run out first (would be completely consumed) if the reaction were to proceed to completion. All other reactants are called excess reactants.

% excess reactant

$$= 100 \, \frac{\text{amount of the excess reactant fed} - \text{amount of the excess reactant required to react with the limiting reactant}}{\text{amount of the excess reactant required to react with the limiting reactant}}$$

Say, $C_7H_{16} + 11O_2 \rightarrow 7CO_2 + 8H_2O$

1 g mol C_7H_{16} and 12 g mol of O_2 are mixed.

∴ Excess reactant: O_2.
Limiting reactant: C_7H_{16}.

If 2 g mol C_7H_{16} and 12 g mol of O_2 are mixed

∴ Excess reactant: C_7H_{16}.
Limiting reactant: O_2.

∴ Amount of product produced is controlled by limiting reactant.

∴ % excess in 1st case $= 100 \times \frac{12-11}{11}$ %

$= \frac{100}{11}$ %

Conversion

Conversion is the fraction of the feed or some key materials in the feed that is converted into products.

$$\% \text{ conversion} = 100 \frac{\text{moles of feed that react}}{\text{moles of feed introduced}}$$

$$C_7H_{16} + 11\,O_2 \rightarrow 7\,CO_2 + 8\,H_2O$$

1 mol C_7H_{16} & 12 mol of O_2 reacted to produce 3.5 moles CO_2 & 4 moles H_2O.

$$\therefore \% \text{ conversion of } C_7H_{16} = \frac{n_{C_7H_{16},0} - n_{C_7H_{16}}}{n_{C_7H_{16},0}} \times 100\%$$

$$= \frac{1 - 0.5}{1} \times 100\%$$

$$= 50\%$$

$$\% \text{ conversion of species } i = \frac{n_{i0} - n_i}{n_{i0}} \times 100\%$$

n_{i0} = moles of feed introduced / or species introduced

n_i = moles of species reactant present after reaction.

$\therefore$ $n_{i0} - n_i$ = moles of species reacted.

Selectivity

selectivity is the ratio of moles of a particular (desired) product produced to moles of another (undesired or by-product) product produced.

$$2\, CH_3OH \rightarrow C_2H_4 + 2\, H_2O$$

$$2\, CH_3OH \rightarrow C_3H_6 + 3\, H_2O$$

∴ At 80% conversion of CH_3OH.

∴ C_2H_4 produced is 19 mol %.

C_3H_6 " " 8 mol %.

∴ selectivity $= \frac{19}{8} = 2.4$ mol C_2H_4/mol C_3H_6

Yield

Yield based on feed: The moles/mass of desired product obtained divided by the moles/mass of the key or limiting reactant feed.

Yield based on reactant consumed: The moles/mass of desired product obtained divided by moles/mass of limiting reactant consumed.

Example

$$C_7H_{16} + 11\,O_2 \rightarrow 7\,CO_2 + 8\,H_2O$$

1 mol of C_7H_{16} & 12 moles O_2 reacted to produce 3.5 moles of CO_2 & 4 moles of H_2O.

$$\%\ \text{yield of } CO_2 = \frac{\text{mass of } CO_2 \text{ produced}}{\text{mass of } C_7H_{16} \text{ consumed}} \times 100$$

$$= \frac{3.5 \times 44}{0.5 \times 100.21} \times 100 \quad \frac{\text{gm } CO_2}{\text{gm } C_7H_{16}}.$$

$$= 307.35\%$$

$$\%\ \text{yield of } CO_2 = \frac{\text{mass of } CO_2 \text{ produced}}{\text{mass of } O_2 \text{ consumed}} \times 100$$

$$= \frac{3.5 \times 44}{5.5 \times 32} \times 100$$

$$= 87.5\% \quad \frac{\text{gm } CO_2}{\text{gm } O_2}.$$

$A + B \rightarrow C$ C is desired reaction

$A + B \rightarrow D$. $\text{yield of } C = \dfrac{\text{mass/moles of } C \text{ produced}}{\text{mass/moles of } A \text{ or } B \text{ consumed}}$.

Moles, density, concentration

Moles: The amount of substance that contains as many elementary entities (6.022×10^{23}) as there are atoms in 0.012 kg of carbon 12. → SI system

A.E 1 lb-mol comprised of
→ $6.022 \times 10^{23} \times 453.6$ molecules.

∴ Molecular weight (MW) → (M) $= \dfrac{\text{Mass}}{\text{mol}}$.

$$\text{g-mol} = \frac{\text{Mass in gm}}{\text{Molecular wt.}}$$

$$\text{lb-mol} = \frac{\text{Mass in lb}}{\text{molecular weight}}$$

$$\frac{100 \cdot \text{gm } H_2O}{} \left| \frac{1 \text{ g-mol } H_2O}{18 \text{ gm } H_2O} \right. = 5.56 \text{ gm-mol.}$$

$$\frac{6 \text{ lb-mol } O_2}{} \left| \frac{32.0 \text{ lb } O_2}{1 \text{ lb mol } O_2} \right. = \underline{192 \text{ lb}} \; O_2$$

$1 \text{ lb mol} = 32 \text{ lb } O_2$.

$1 \text{ gm mol} = 32 \text{ gm } O_2$.

$1 \text{ kg-mol} = 32 \text{ kg } O_2$.

If a bucket of NaOH holds 2.00 lb of NaOH.

$2 \text{ lb NaOH} = \frac{2}{40} \text{ lb-mol NaOH}$

$= 0.05$ "

$$\frac{2 \text{ lb NaOH}}{} \left| \frac{1 \text{ lb mol NaOH}}{40 \text{ lb NaOH}} \right| \frac{454 \text{ gm mol.}}{1 \text{ lb mol.}} = 22.7 \text{ gm mol.}$$

$1 \text{ lb mol} = 454 \text{ gm-mol.}$

References

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