IC 211 CHEMICAL STOICHIOMETRY

Introduction to Engineering Principles and units

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Recommended Books and References Used

1. David. M. Himmerblau and James B. Riggs ***"Basic Principles and Calculations in Chemical Engineering"***, 7th edition.

2. C J Geankoplis, (4th Edition), 2003, *"**Transport Process and Separation Process Principles**"*, Pearson Education LTD.

3. กัญจนา บุณยเกียรติ (พิมพ์ครั้งที่ 5) (พ.ศ.2543), ***"การคำนวณขั้นต้น ในวิชาวิศวกรรมเคมี"***, สำนักพิมพ์แห่งจุฬาลงกรณ์มหาวิทยาลัย.

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Contents

1.Introduction

- Introduction to the course
- Introduction to chemical stoichiometry for industrial process

2.Basic Calculation for Engineering

- Unit and dimension of selected system, e.g. temperature, pressure, force, energy, density and composition.

3.Gases

- Rules that used to explain gas behaviour.
- Ideal and real (non-ideal) gas.

4. Fluid Flow

- An introduction

1. Introduction

-Example of industrial process : *How Glass Bottles are Made (youtube video; by Education World).*

- Most of the industrial process may start from the initial experiment in a laboratory, though there is a huge difference between those two places, which is a scale of production. (Larger scale is necessary for an industrial production)

- The calculation is done as a whole process, but it could be calculated separately as an individual unit, for example raw material unit, melting unit and forming unit.

1. Introduction

-The basic calculation is done for the MOMENTUM, HEAT and MASS TRANSFER of each individual units.

- The basic ideas for calculation of the momentum, heat and mass transfer are the “Equilibrium of Mass” and the “Equilibrium of Energy” using the “Mass Conservation Law and Energy Conservation Law”.

- To control and develop the process in the industry these mass and energy calculation are importance.

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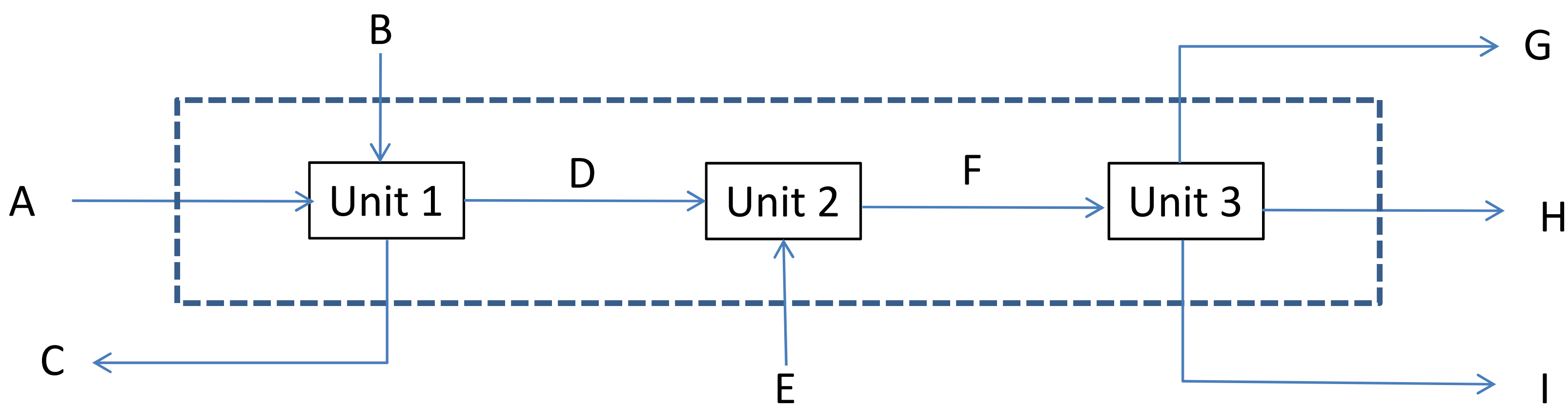
2.1 Technique of Problem Solving

- The technique suggested for the solving of engineering problem in chemical engineering are as follow;

1. Try to understand the problem, find what is needed.
2. Try to see what are the extra information needed. Find them.
3. Draw the “Flow Chart” or “Block Diagram” of the system showing the process where the transportation of stream in the system presents.



4. Pick the "***Basis***" on which to start the problem.

5. Write down the *balanced* chemical equation (if involves).

6. Decide what principles, formulas that are controlling the problem and what types of calculation you will use. If there are many choice, select one with the most suitable for the process. If there is an unknown parameter, leaves it as a letter (e.g. x, c) and think as we can solve the problem if we know the value of that parameter.

7. Be careful during the calculation, e.g. checking that the units present are correct.

8. Consider if the answer you are getting is reasonable.

2.2 Units and Dimensions

"Dimension" : basic concepts of measurement, e.g. length, time, mass and temperature.

"Units" : the means of expressing the dimensions, e.g. feet, minute, kilogram and Celsius.

Benefits of Using Units →

1. Reduce the possible of errors in the calculation.
2. Reduce intermediate calculations and time of solving.
3. Help for understanding the formula rather than remember it.
4. Easy interpretation of physical meaning of the number.

Systems of Units

"SI unit" : Le Systeme Internationale d'Unites (international

system.

"AE" : American Engineering System of Units

"USCS" : U.S. Conventional System

"Metric Systems" : CGS (centimeters, grams, seconds)

"English System"

why the units are so important in the engineering calculations ?

→ 1.9 g/min + 2.0 L/s =?

→ 2 seconds + 5 kilogram =?

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	
Mass	tonne, ton (Mg), gram	t, g	

* Symbols for units do not take a plural form, but plural forms are used for the unabbreviated names. Non-SI units such as day (d), liter or litre (L), and ton or tonne (t) are legally recognized for use with SI.

TABLE 1.3 SI Prefixes

Factor	Prefix	Symbol	Factor	Prefix	Symbol
10^9	giga	G	10^{-1}	deci	d
10^6	mega	M	10^{-2}	centi	c
10^3	kilo	k	10^{-3}	milli	m
10^2	hecto	h	10^{-6}	micro	μ
10^1	deka	da	10^{-9}	nano	n

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 of Units

1. Addition, Subtraction and Equality

   → *only if the associated units are the same.*

Consider : 5 kg + 6 J, 5 pounds + 150 grams , 5 cm + 10 cm

2. Multiplication and Division

   → *can do the operations, even if the units are not the same.*

   → *But !! Resulting in the new unit.*

Consider : 5 Litters ÷ 2 seconds = 2.5 L/s , 5 L / 5 L = 1 L

Conversion of Units and Conversion Factors

In order to do the calculation to solve the engineering problems, system of unit has to be the same for all units present in the equation. → What is the total cost of the chemical you have bought? If you bought sodium carbonate 500 Baht from Thailand and copper sulphate 125 $ from USA. (Currency exchange 1 $ is about 30 baht)

→Prefer format for unit conversion

$$= \frac{500\ \cancel{\text{Baht}}}{} \left| \frac{1\ \$}{30\ \cancel{\text{Baht}}} \right. = 16.6\ \$$$

Then do other calculation….

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?

2 x 1100 ft	1 mi	60 s	60 min
s	5280 ft	1 min	1 hr

Exercise :

1. Convert 2 km to miles (1 mile = 1.61 km)

2. Convert 400 in.^{3}/day to cm^3/min (1 in = 2.54 cm)

3. The particle size of ZnS is about 1.8 nm, what is the size in decimeter (dm).

Special attention!!!

Newton's Law : $F = ma$, this really comes from $F = Cma$

where F = force

C = Constant whose numerical value and units are depending on the F, m and a.

m = mass

a = acceleration

Why in SI system → the C is ignored

In SI unit, the force is defined to be the Newton (N) when 1 kg is accelerated at 1 m/s^2. C will then = 1 $N/(kg)(m/s^2)$, which could be ignore as it = 1.

Special attention!!! Mass and Force

Weight is actually a Force (F = Cma or Cmg)

In AE system, force unit is in lb_f (poundforce), in which the definition is mass of 1 lb_m is accelerated at g ft/s^2 (about 32.2 ft/s^2 depending on the place of the mass).

$$F = \underbrace{\left(\frac{1(\text{lb}_f)(s^2)}{32.174(\text{lb}_m)(\text{ft})}\right)}_{\tilde{C}}\left(\frac{\underbrace{1\ \text{lb}_m}_{\tilde{m}}}{}\middle|\frac{\underbrace{g\ \text{ft}}_{\tilde{g}}}{s^2}\right) = 1\ \text{lb}_f$$

The inverse of the C is converted to g_c, where

$$g_c = 32.174\frac{(\text{ft})(\text{lb}_m)}{(\text{s}^2)(\text{lb}_f)}$$

g_c = conversion factor

(used to cancel some units)

Remember !! Weight $\neq$ mass , as weight is a force.

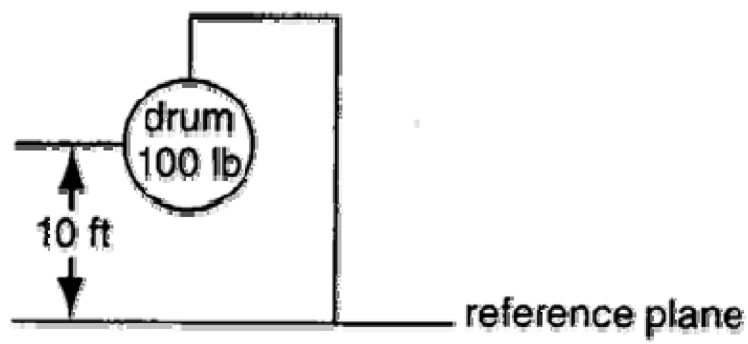
Exercise : What is a g_c in when g = 9.80665 m/s^2?

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

Solution 1. read question and find unknown paramenter

2. what are known quantities?

3. How are they related? (P = mgh)



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

Dimensional Consistency (Homogeneity)

"Equation must be dimensionally consistent"

Consider : $A = B + C - D$

and $X = W \times Y^2 / Z$

Which term in these equation must be the same?

Exercise : From the equation $d = 16.2 - 16.2e^{-0.021t}$

d is dept in **micron** (μm) and ***t*** is time in **second**.

Change this equation to that you could express the idea in **inch** and **minute** for d and t, respectively.

Solution : → ***d*** is a function of ***t***

→ ***unit*** *of right-hand side* of the equation should have a dimension of ***Length***. *Thus 1st* ***16.2*** *has micron unit as well as* $\mathbf{16.2e^{-0.021t}}$.

→ *the exponential term** $\mathbf{e^{-0.021t}}$ must be dimensionless, which leads 0.021 must have the unit of s^{-1} (to eliminate time dimension)

$$d_{\text{in}} = \frac{16.2\ \mu\text{m}}{} \bigg| \frac{1\ \text{m}}{10^6\ \mu\text{m}} \bigg| \frac{39.27\ \text{in.}}{1\ \text{m}} \left[1 - \exp \frac{-0.021}{s} \bigg| \frac{60 s}{1\ \text{min}} \bigg| \frac{t_{\text{min}}}{} \right]$$

$$= 6.38 \times 10^{-4}(1 - e^{-1.26 t_{\text{min}}})\ \text{inches}$$

*** Nonlinear function, e.g. log, exponential and sin, should have dimensionless before processing a calculation.**

Exercise : Is the following equation homogeneity?

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

-Sometimes the group of symbol that put together due to the theoretical or experimental base, it might be ***“dimensionless”*** or ***“nondimensional group”***. For example, Reynolds Number (N_{RE}) in fluid mechanic.

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

D : pipe diameter (length)

ν : fluid velocity (length/time)

ρ : density (mass/volume)

μ : viscosity (mass /length · time)

$$\frac{cm}{}\bigg|\frac{cm}{s}\bigg|\frac{g}{cm^3}\bigg|\frac{(cm)\,(s)}{g}$$

Significant Figure

The scale of the accuracy of the results from the calculation depends on the application of that results. For example, "*cooking ingredient* and *laboratory composition*" or "*engineering calculation* and *amount of fertilizer* used for the lawn.

If the cost of inaccuracy is huge (failure, fire, downtime, etc.), the degree of uncertainty is very important.

Several ways to consider degree of certainty of number, i.e.

1) common sense
2) absolute error
3) relative error
4) statistical error

Absolute error

Case 1) numbers with a decimal point

Case 2) number without a decimal point

Case 1 → last significant figure represents the associated uncertainty.

e.g. 100.3 → range from 100.25 – 100.35 (±0.05)

100.3**00** → 6 significant figures

→ there is a reason to display this

→ may be it is rounded from 100.2997

Case 2 → e.g. 201,3**00** has only 4 significant figures.

Operations of significant figure

Multiply or dividing

- Result obtained from the operations must retain the lowest significant figure.

e.g. (1.47)(3.0926) = 4.54612 → ANS 4.55

Add or subtract

- Result must retain the lowest number of decimal places.
- Final significant figures determined by the error interval of the largest number.

e.g. 110.3+0.038 = 110.338 →ANS 110.3

Upper Bound	Lower Bound
$110.3 + 0.05 = 110.35$	$110.3 - 0.05 = 110.25$
$0.038 + 0.0005 = 0.0385$	$0.038 - 0.005 = 0.0375$
110.3885	110.2875

The midpoint of these two numbers is 110.338.

Relative Error

- Consider 1.01/1.09 = 0.9266 → then you answer 0.92**7**

- calculate the error of the answer by

0.00**1**/0.92**7** x 100 → 0.1% , then compare with the error of the larger number by 0.0**1**/1.0**9**) x 100 → about 1% uncertainty.

- Let's fix the error at about 1% → so the answer should be 0.93 instead.

Statistical Error

- is more complicated as the statistical calculation is needed, which includes the "confidence limit" or "consideration of error propagation" during each steps of calculation.

Validation / Verification of Problem Solution

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

Home Work

Page 33 in Himmelblau and Riggs Text book

*	1.2
**	1.7
**	1.12
***	1.21
***	1.23
*	1.28
*	1.34

2.3 Mole, Density and Concentration

Mole

Mole is a certain amount of material corresponding to a specified number of molecule, atoms, electrons or other types of particles.

Mole in SI unit → composes of 6.02×10^{23} molecules

(Avogadro's Number)

How about ***pound mole***? → = $453.6 \times (6.02 \times 10^{23})$ molecules

How about ***kilogram mole***? → = $1000 \times (6.02 \times 10^{23})$ molecules

Thus, we usually write down ***"mole"*** as ***"g mole"***.

<u>**Mole**</u>

How to convert ***"mole"*** to ***"mass"*** and *vice versa*?

<u>Consider</u> g mole, lb mole and kg mole

e.g. Carbon → atomic mass = 12.xx g /mole

→g mole mass = 12 g

→lb mole mass = 453.6 x 12 g

(453.6 x g mole)

$$= \frac{453.6\text{x}12 \text{ g}}{} \left| \frac{1 \text{ lb}}{453.6 \text{ g}} \right| = 12 \text{ lb}$$

→ Kg mole? = (1000 x g mole)

Mole

How to convert ***"mole"*** to ***"mass"*** and *vice versa*?

→Make a use of *"Molecular weight"* – which is a mass per mole.

$$\text{molecular weight (MW)} = \frac{\text{mass}}{\text{mole}}$$

Thus,

$$\text{the g mol} = \frac{\text{mass in g}}{\text{molecular weight}}$$

$$\text{the lb mol} = \frac{\text{mass in lb}}{\text{molecular weight}}$$

$$\text{mass in g} = (\text{MW})(\text{g mol})$$

$$\text{mass in lb} = (\text{MW})(\text{lb mol})$$

Mole

e.g. 100 g of water = ? g mole.

$$\frac{100.0 \text{ g } H_2O}{} \bigg| \frac{1 \text{ g mol } H_2O}{18.0 \text{ g } H_2O} = 5.56 \text{ g mol } H_2O$$

e.g. 6 lb mole of oxygen gas = ? pounds.

$$\frac{6.0 \text{ lb mol } O_2}{} \bigg| \frac{32.0 \text{ lb } O_2}{1 \text{ lb mol } O_2} = 192 \text{ lb } O_2$$

e.g. If a bucket holds 2.00 lb of NaOH, how many

a) Pound mole of NaOH ?

b) Gram moles of NaOH ?

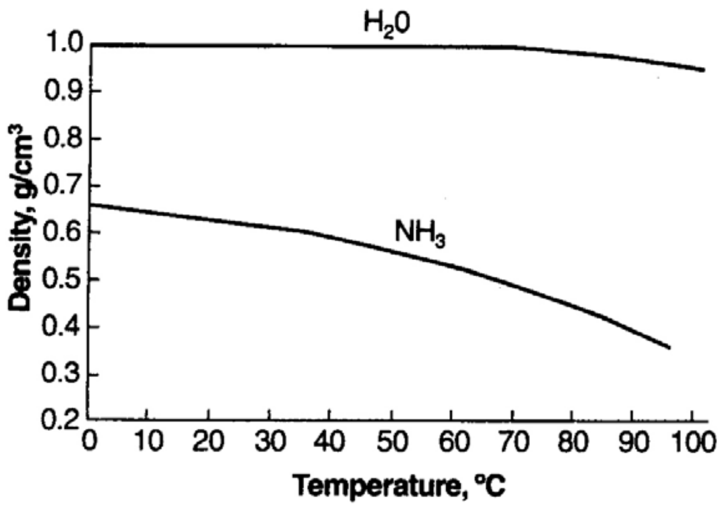
Ans. (a) 0.050 lb mol NaOH, (b) 22.7 g mol

****** g mole, lb mole and kg mole are the unit of mole NOT a mass********

Density

"Density" ρ is a ratio of mass per unit volume. (m/v)

"Specific Volume" $\hat{V}$ is a reverse of density. (v/m)



Temperature and Pressure have effect on the density (Temperature has stronger effect, esp. for liquid). But here we ignore these effects at the moment.

Other relevant quantities are;

Molar density = ρ / MW and Molar Volume = MW / ρ

Density

→ "Bulk Density" ρ_B is considered in a packed bed of particles containing a void spaces, the bulk density is then;

$$\rho_B = \text{bulk density} = \frac{\text{total mass of solids}}{\text{total empty bed volume}}$$

→ "Density of mixture or solution" could be calculated by

$$V = \sum_{i=1}^{n} V_i \qquad \text{where } n = \text{number of components}$$

$$m = \sum_{i=1}^{n} m_i$$

$$\rho_{\text{solution}} = \frac{m}{V}$$

Example : An empty 10 gal tank weights 4.5 lb. What is the total weight of the tank plus the water when it is filled with 5 gal of water?

Example : An empty 10 gal tank weights 4.5 lb. What is the total weight of the tank plus the water when it is filled with 5 gal of water?

Solution : take the density of water = 1000 kg/m^3

total mass = mass of tank + mass of water

$$= 4.5\text{ lb} + \left(\frac{1000\text{ kg}}{\text{m}^3} \,\Bigg|\, 5\text{ gal} \,\Bigg|\, \frac{3.78\times10^{-3}\text{ m}^3}{1\text{ gal}} \,\Bigg|\, \frac{1\text{ lb}}{4.536\times10^{-1}\text{ kg}} \right)$$

= 4.5 lb + 41.7 lb

= 46.2 lb

Specific gravity

The ratio of two densities, esp. of the interesting substance A and the reference.

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

Common used references

- Liquids and solids
  - Reference substance → water

    (1.000 g/cm^3, 1000 kg/m^3, 62.43 lb/ft^3 at **4 ^{o}C**)
- Gases
  - Reference substance → air or others

To be precise when report the sp.gr. should be reported with the temperature, e.g.

$$\text{sp. gr.} = 0.73\frac{20^o}{4^o}$$

Specific gravity

sp.gr. In a petroleum industry, it is reported in term of hydrometer scale, so called °API (American petroleum industry.

$$^{o}\text{API} = \frac{141.5}{\text{sp. gr. } \dfrac{60^{o}\text{F}}{60^{o}\text{F}}} - 131.5$$

$$\text{sp. gr.} \frac{60^{o}\text{F}}{60^{o}\text{F}} = \frac{141.5}{^{o}\text{API} + 131.5}$$

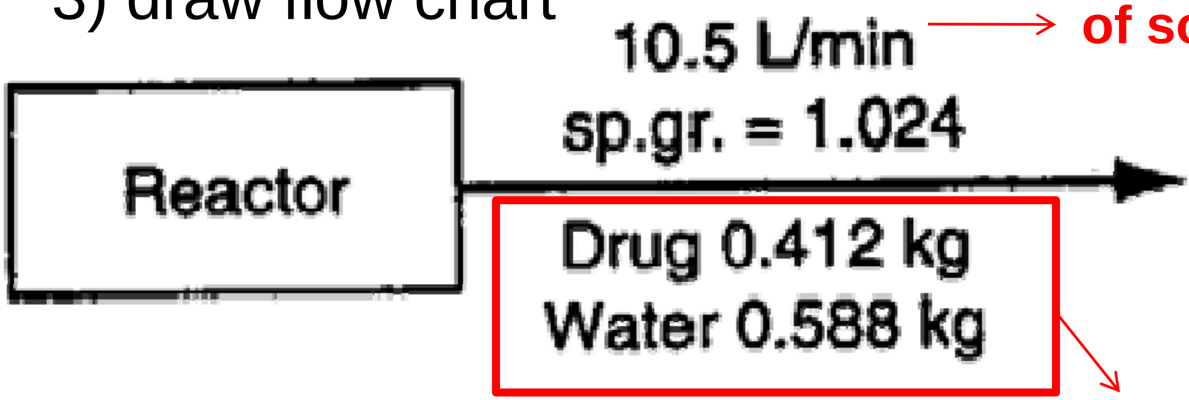
Other existing unit for sp.gr. → (Baume, ^{o}Be), (Twaddel, ^{o}TW)

Example : In the production of a drug having a molecular weight of 192, the exit stream from the reactor flows at a rate of **10.5** L/min. The drug concentration is **41.2%** (in water), and the specific gravity of the solution is **1.024**. Calculate the concentration of the drug (in kg/L) in the exit stream, and the flow rate of the drug in kg mol/min.

Solution : 1) what is/are the question?

2) what have been provided? What else is needed?

3) draw flow chart



of solution

How about 412 kg of drug and 588 kg of water?

4) choose the "Basis". → 1 kg of solution

4) do the calculation.

basis

Next convert the amount of drug in 1.000 kg of solution to mass of drug per volume of solution using the density

$$\frac{0.412 \text{ kg drug}}{1.000 \text{ kg soln}} \left| \frac{1.024 \text{ g soln}}{1 \text{ cm}^3} \right| \frac{1 \text{ kg}}{10^3 \text{ g}} \left| \frac{10^3 \text{cm}^3}{1 \text{ L}} \right. = 0.422 \text{ kg drug/L soln}$$

sp.gr.

Basis → 1 minute

thus from the problem:10.5 L/min of solution, you will then get

$$\frac{10.5 \text{ L soln}}{1 \text{ min}} \left| \frac{0.422 \text{ kg drug}}{1 \text{ L soln}} \right| \frac{1 \text{ kg mol drug}}{192 \text{ kg drug}} = 0.023 \text{ kg mol/min}$$

HW 3

1. If a 70% (by weight) solution of glycerol has a specific gravity of 1.184 at 15 ^{o}C, what is the density of the solution in (a) g/cm^3? (b) lb$_m$/ft^3? And (c) kg/m^3?

2. The specific gravity of steel is 7.9. What is the volume in cubic feet of a steel ingot weighing 4000 lb?

3. A solution in water contains 1.704 kg of HNO_3/kg H_2O, and the solution has a specific gravity of 1.382 at 20 ^{o}C. What is the mass of HNO_3 in kg per cubic meter of solution at 20 ^{o}C?

Mole fraction, Mass (weight) Fraction

“***Mole Fraction***” is a number of moles of an interesting compound in the mixture of compound or solution divide by the total number of moles.

$$\text{mole fraction of } A = \frac{\text{moles of } A}{\text{total moles}}$$

$$\text{mass (weight) fraction of } A = \frac{\text{mass of } A}{\text{total mass}}$$

Mole % and Mass or (weight) % could be calculated by x 100 to the mole and mass (weight) fraction, respectively.

Example : An industrial-strength drain cleaner contains 5.00 kg of water and 5.00 kg of NaOH. What are the mass (weight) fractions and mole fractions of each component in the drain cleaner container?

Solution :

Basis: 10.0 kg of total solution

Component	kg	Weight fraction	Mol. Wt.	kg mol	Mole fraction
H_2O	5.00	$\frac{5.00}{10.0} = 0.500$	18.0	0.278	$\frac{0.278}{0.403} = 0.69$
NaOH	5.00	$\frac{5.00}{10.00} = 0.500$	40.0	0.125	$\frac{0.125}{0.403} = 0.31$
Total	10.00	1.000		0.403	1.00

The kilogram moles are calculated as follows:

$$\frac{5.00 \text{ kg } H_2O}{} \left| \frac{1 \text{ kg mol } H_2O}{18.0 \text{ kg } H_2O} \right. = 0.278 \text{ kg mol } H_2O$$

$$\frac{5.00 \text{ kg NaOH}}{} \left| \frac{1 \text{ kg mol NaOH}}{40.0 \text{ kg NaOH}} \right. = 0.125 \text{ kg mol NaOH}$$

Concentration

a) Mass per unit volume e.g. lb of solute/ft^3 of solution

b) Mole per unit volume e.g. g mole of solute/L

c) Part per million (ppm), Part per billion (ppb)→extremely dilute

d) Part per million by volume (ppmv), part per billion by volume (ppbv)

e) Other e.g. molality, normality, g mole/L etc.

Sufficient to cause death

Occupational safety and health administration

Example : The current OSHA 8-hour limit for HCN in air is 10.0ppm. A lethal dose of HCN in air is (from the Merck Index) 300 mg/kg of air at room temperature. How many mg HCN/kg of air is 10.0 ppm? What fraction of the lethal dose is 10.0 ppm?

Solution : **Basis: 1 kg mol of the air/HCN mixture**

Draw a simple picture. Put the data in the figure.

$$\text{The 10.0 ppm is } \frac{10.0 \text{ g mol HCN}}{10^6(\text{air} + \text{HCN})\text{g mol}} = \frac{10.0 \text{ g mol HCN}}{10^6 \text{ g mol air}}$$

Then use MW of HCN (=27.03) and air (=29) to convert the g mole to mass.

$$\frac{10.0 \text{ g mol HCN}}{10^6 \text{ g mol air}} \left| \frac{27.03 \text{ g HCN}}{1 \text{ g mol HCN}} \right| \frac{1 \text{ g mol air}}{29 \text{ g air}} \left| \frac{1000 \text{ mg HCN}}{1 \text{ g HCN}} \right| \frac{1000 \text{ g air}}{1 \text{ kg air}}$$

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

*** Merck ➔ 300 mg HCN/kg air*

Then calculate the fraction as;

$$\frac{9.32}{300} = 0.031$$

Flow rate

In a continuous process, the flow rate is a transportation of material stream through a pipe.

- Mass flow rate $$\dot{m} = \frac{m}{t}$$

- Volumetric flow rate $$F = \frac{V}{t}$$

- Molar flow rate $$\dot{n} = \frac{n}{t}$$

Exercise: Forty gal/min of a hydrocarbon fuel having a specific gravity of 0.91 flow into a tank truck with a load limit of 40,000 lb of fuel. How long will it take to fill the tank in the truck?

Exercise: Pure chlorine enters a process. By measurement it is found that 2.4 kg of chlorine pass into the process every 3.1 minutes. Calculate the molar flow rate of the chlorine in kg mol/hr.

Home Work

Page 69 in Himmelblau and Riggs Text book

*	2.11
*	2.13
**	2.19
**	2.33
**	2.38
*	2.46
*	1.52

2.4 Choosing a basis

-is a reference used by you for a calculation you plan to make.
-may be a mass (e.g. 5 kg), a volume (1 L), a flow rate or else.

Think about

a. What do I have to start with? (what are provided)

b. What answer is call for? (question is?)

c. What is the most convenient basis to use? (e.g. if the ***mole fractions*** of material are provided. Then you may select ***100 kg mole*** as a basis. On the other hand, if the ***mass fractions*** are known, then take ***100 kg*** as a basis. If the problem asks for the ***rate***, the ***time*** might be the best "basis".

Always state the basis you have chosen for your calculations by writing it prominently on your calculation sheets (or computer screen).

The dehydration of the lower alkanes can be carried out using a ceric oxide (CeO) catalyst. What is the mass fraction and mole fraction of Ce and O in the catalyst?

Solution

Start the solution by selecting a basis. Because no specific amount of material is specified, the question what do I have to start with does not help decide on a basis. Neither does the question about the desired answer. Thus, selecting a convenient basis becomes the best choice for a basis. What do you know about CeO? You know from the formula that one mole of Ce is combined with one mole of O. Consequently, a basis of 2 kg mol (or 2 g mol, or 2 lb mol, etc.) would make sense. You can get the atomic weights for Ce and O from Appendix B, and then you are prepared to calculate the respective masses of Ce and O in CeO. The calculations are presented in the form of the following table:

Basis: 2 kg mol of CeO

Component	kg mol	Mole fraction	Mol. wt.	kg.	Mass fraction
Ce	1	0.50	140.12	140.12	0.90
O	1	0.50	16.0	16.0	0.10
Total	2	1.00	156.1	156.1	1.00

2.5 Temperature

°F → Fahrenheit °R → Rankine

°C → Celsius ***K* → *Kelvin***

$$\Delta°F = \Delta°R$$

$$\Delta°C = \Delta K$$

$$T_{°R} = T_{°F}\left(\frac{1\ \Delta°R}{1\ \Delta°F}\right) + 460°R$$

$$T_{K} = T_{°C}\left(\frac{1\ \Delta K}{1\ \Delta°C}\right) + 273\ K$$

$$\frac{\Delta°C}{\Delta°F} = 1.8 \quad \text{or} \quad \Delta°C = 1.8\ \Delta°F$$

$$\frac{\Delta K}{\Delta°R} = 1.8 \quad \text{or} \quad \Delta K = 1.8\ \Delta°R$$

$$T_{°F} - 32°F = T_{°C}\left(\frac{1.8\ \Delta°F}{1\ \Delta°C}\right)$$

$$T_{°C} = (T_{°F} - 32°F)\left(\frac{1\ \Delta°C}{1.8\ \Delta°F}\right)$$

e.g. Convert 100 °C to K, °F and °R.

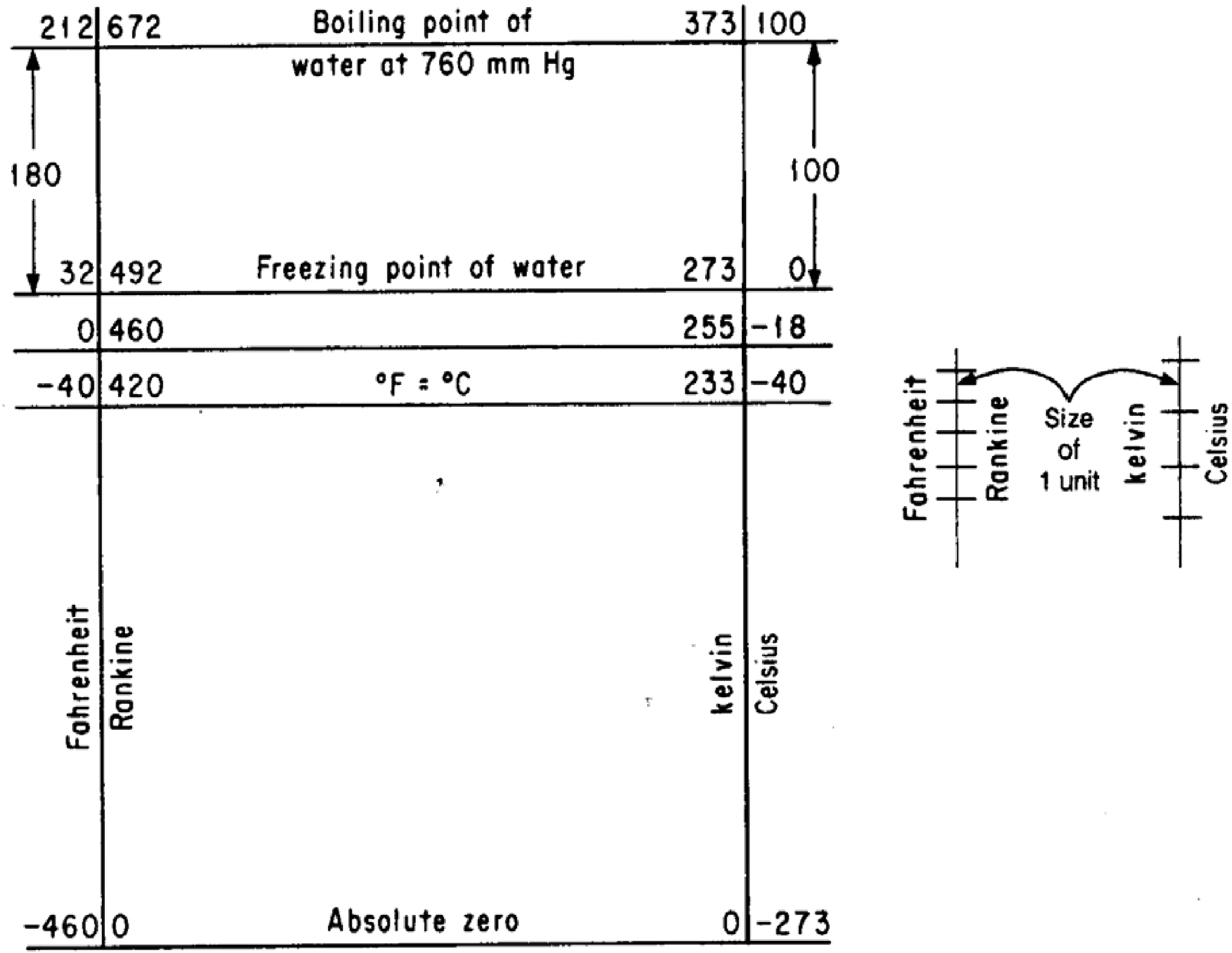
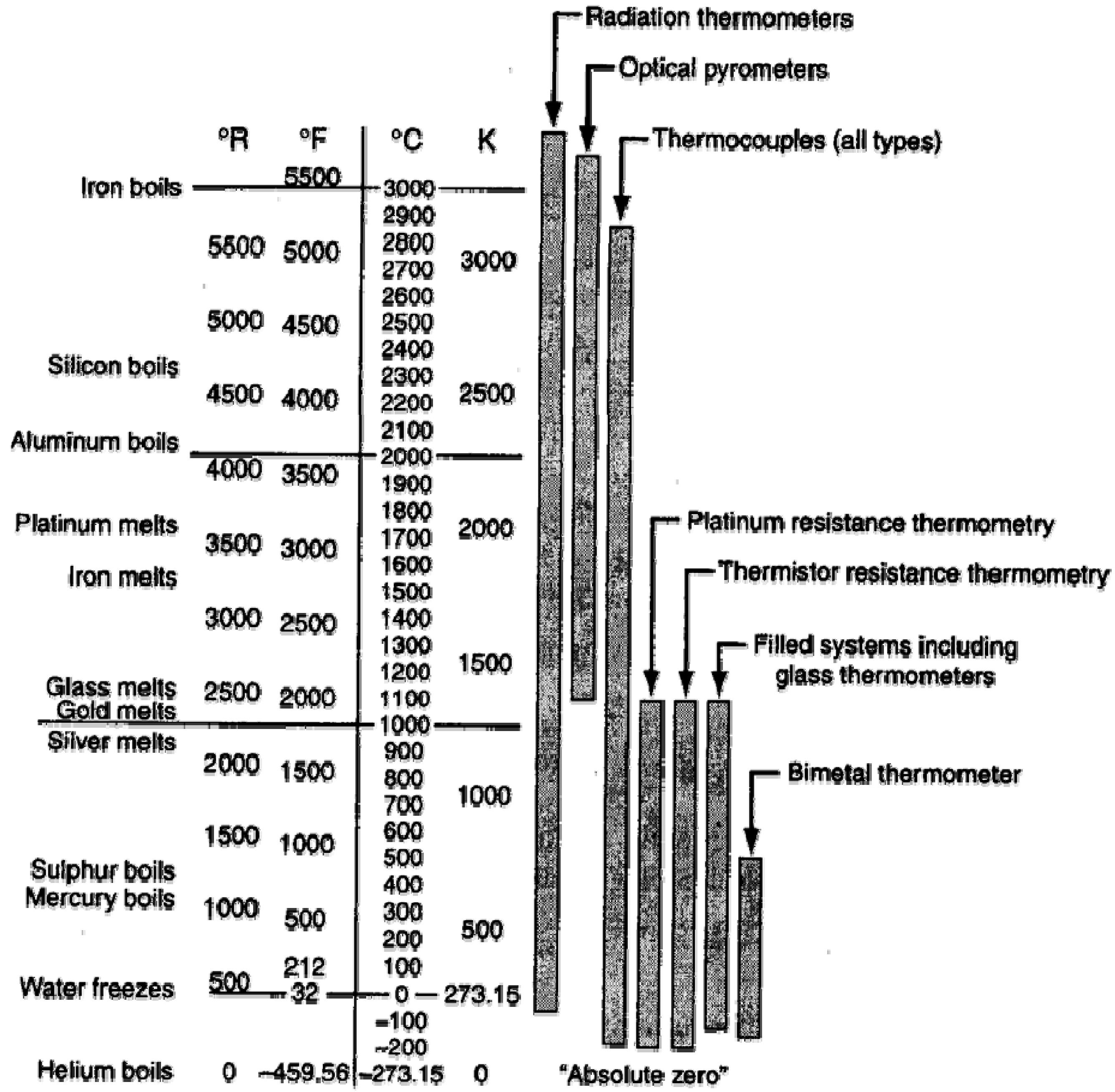


Figure 4.1 Temperatures scales.

Temperature measuring instruments



2.5 Temperature

Δ°C, Δ°F, ΔK and Δ°R are not in the standard use. Thus some other books try to distinguish these from the degree units.

Difference between temperature dregrees → °C, °F, …

Degree units → C°, F°, …

But these are rarely used. Thus when you see!! the temperature unit in the equation or constant, bare in mind that it may be a (1) difference of temperature or (2) temperature unit.

<u>Consider:</u>

1. ***"Heat capacity" (in chapter 21 of the 1st reference book)*** has the unit of **J/(g mole)(K)**. Is "K" an interval in temperature (ΔK) or any actual temperature (K)?

→ <u>ANS</u> ΔK

2. ***"Gas constant" (R)*** has the unit of **(kg)(m^2)/(kg mole)(s^2)(K)**. What does K actually mean?

→ <u>ANS</u> K (absolute temperature)

*** just go back to the principle that explain both terms.*

Exercise:

1.Consider this following equation, then state the unit of the number ***a*** an ***b***.

$$T_{°F} = a + bT_{°C}$$

Solution : ***a*** must be in a unit of °F and

b must be in a unit that relevant to $°C^{-1}$ (but not that simple) → use this relationship Δ°F = (Δ°C)/(1.8).

2. The heat capacity of sulfuric acid has the unit of J/(g mol)(°C), and is given by the relation

Heat capacity = 139.1 + 1.56 x 10^{-1}***T*** ,where ***T*** is expressed in °C

Modify the formula so that the unit is converted to Btu/(lb mol)(°R).

Solution Heat capacity [unit J/(g mol)(°C)] = $139.1 + (1.56 \times 10^{-1})\boldsymbol{T}$

The symbol °C in the denominator of the heat capacity stands for the unit temperature difference, Δ°C, not the temperature, whereas the units of T in the equation are in °C. First you have to substitute the proper equation in the formula to convert T in °C to T in °R, and then by multiplication by conversion factors convert the units on the righthand side of the equation to Btu/(lb mol) (°R) as requested.

$$\text{heat capacity} = \left\{139.1 + 1.56 \times 10^{-1} \overbrace{\left[(T_{°R} - 460 - 32)\frac{1}{1.8}\right]}^{T_{°C}}\right\}$$

$$\times \frac{1\ \text{J}}{(\text{g mol})(°\text{C})} \underbrace{\left|\frac{1\ \text{Btu}}{1055\ \text{J}}\right|\frac{454\ \text{g mol}}{1\ \text{lb mol}}\left|\frac{1°\text{C}}{1.8°\text{R}}\right.}_{\text{conversion factors}} = 23.06 + 2.07 \times 10^{-2} T_{°R}$$

Note the suppression of the Δ symbol in the conversion between Δ°C and Δ°R.

Home Work

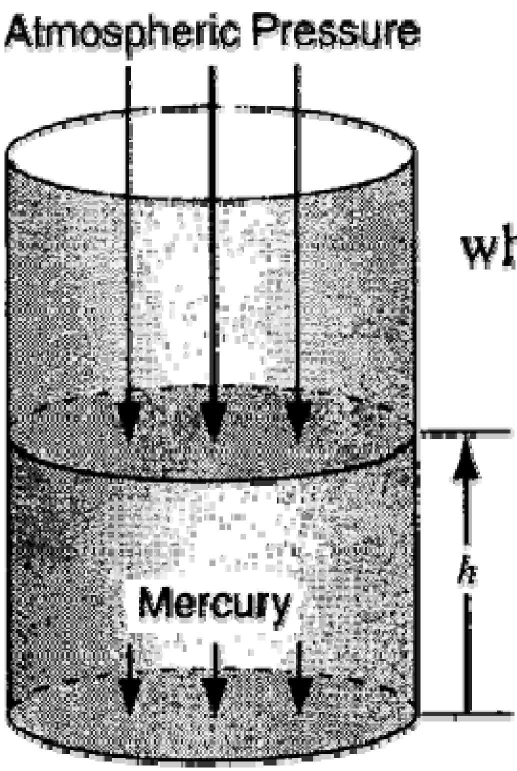
Page 97 in Himmelblau and Riggs Text book

- * 4.3
- ** 4.4
- ** 4.9

2.6 Pressure

"Pressure" : a normal force (usually perpendicular) per unit area.

<u>Consider: </u>the pressure at the bottom of the static column of mercury



$$p = \frac{F}{A} = \rho g h + p_0$$

F=Cma or *F=ma*
a=g, in this case
Density = m/v

where p = pressure at the bottom of the column of the fluid
F = force
A = area
ρ = density of fluid
g = acceleration of gravity
h = height of the fluid column
p_0 = pressure at the top of the column of fluid

2.6 Pressure

Get used to these units of pressure!!!

<u>SI system</u> *(force → N, area → m^2 then N/m^2 = Pa)*

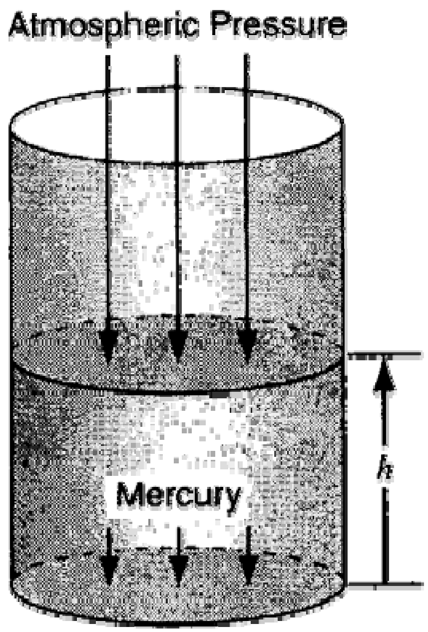
1. 100 kPa = 1 bar
2. Kg_f/cm^2 → very common but not standard use SI system
3. 760 Torr = 1 atm

<u>AE system</u>

1. mm Hg (millimeters of mercury)
2. in. Hg (inches of mercury)
3. ft H_2O (feet of water)
4. in. H2O (inches of water)
5. atm (atmospheres)
6. psi (pound (force) per square inch (lb_f/in^2)

Example:

Calculate the pressure at the bottom of the open column containing liquid mercury ;
Liquid is mercury, which has ρ = 13.55 g/cm^3.
Area of the column is 1 cm^2 and the height of liquid is 50 cm.



Solution :

$$P = F/a + \mathbf{P_0} = \rho g h + \mathbf{P_0}$$

$$F = ma = mg$$

$$m = v\rho$$

density, g, h, area

$$F = \frac{13.55\ \text{g}}{\text{cm}^3} \left| \frac{980\ \text{cm}}{\text{s}^2} \right| \frac{50\ \text{cm}}{} \left| \frac{1\ \text{cm}^2}{} \right| \frac{1\ \text{kg}}{1000\ \text{g}} \left| \frac{1\ \text{m}}{100\ \text{cm}} \right| \frac{1(\text{N})(\text{s}^2)}{1(\text{kg})(\text{m})}$$

$$= 6.64\ \text{N}$$

volume

Conversion factor

Solution (cont.) : $P = F/A + \mathbf{P_0} = \rho g h + \mathbf{P_0}$

$F = ma = mg$

$m =$ What is the equivalent pressure to 60 Gpa in

(a) atmospheres
(b) psia
(c) inches of Hg
(d) mm of Hg

Then $P = F/A + P_0$

Force (F)

$$p = \frac{6.64\ \text{N}}{1\ \text{cm}^2}\left|\left(\frac{100\ \text{cm}}{1\ \text{m}}\right)^2\right|\frac{(1\ \text{m}^2)(1\ \text{Pa})}{(1\ \text{N})}\left|\frac{1\ \text{kPa}}{1000\ \text{Pa}}\right. + \boxed{p_0} = 66.4\ \text{kPa} + p_0$$

Area (A)

Conversion factor

<u>Example :</u> What is the equivalent pressure to 60 Gpa in
a) atmospheres, b) psia, c) inches of Hg and d) mm of Hg

Solution :

For the solution, use the standard atmosphere.

Basis: 60 GPa

(a) $$\frac{60\ \text{GPa}}{} \bigg| \frac{10^6\ \text{kPa}}{1\ \text{GPa}} \bigg| \frac{1\ \text{atm}}{101.3\ \text{kPa}} = 0.59 \times 10^6\ \text{atm}$$

(b) $$\frac{60\ \text{GPa}}{} \bigg| \frac{10^6\ \text{kPa}}{1\ \text{GPa}} \bigg| \frac{14.696\ \text{psia}}{101.3\ \text{kPa}} = 8.70 \times 10^6\ \text{psia}$$

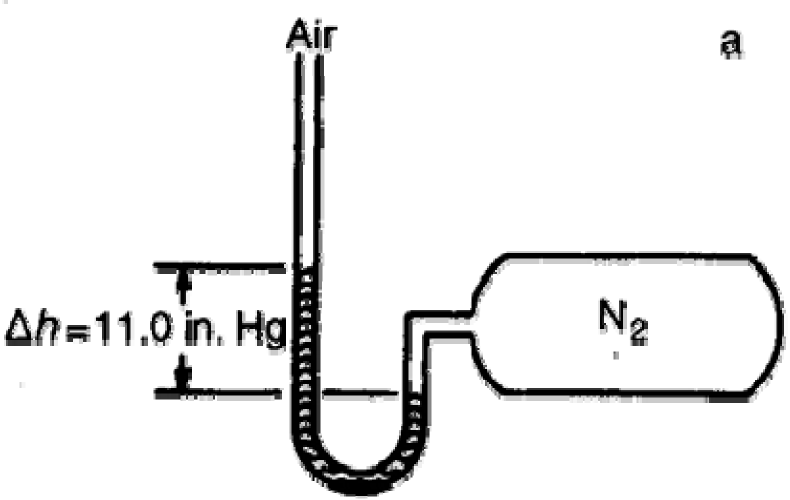
(c) $$\frac{60\ \text{GPa}}{} \bigg| \frac{10^6\ \text{kPa}}{1\ \text{GPa}} \bigg| \frac{29.92\ \text{in. Hg}}{101.3\ \text{kPa}} = 1.77 \times 10^7\ \text{in. Hg}$$

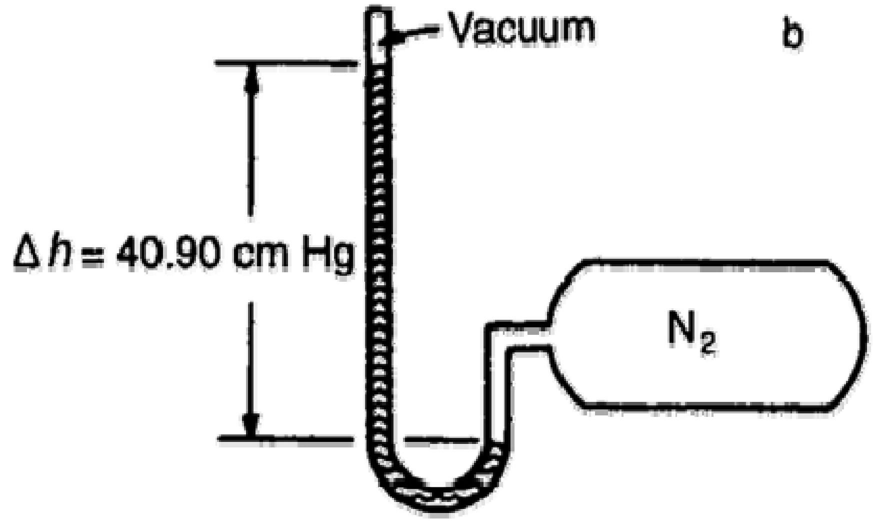
(d) $$\frac{60\ \text{GPa}}{} \bigg| \frac{10^6\ \text{kPa}}{1\ \text{GPa}} \bigg| \frac{760\ \text{mm Hg}}{101.3\ \text{kPa}} = 4.50 \times 10^8\ \text{mm Hg}$$

Measurement of Pressure

Pressure could be expressed as “relative pressure” or

“absolute pressure”





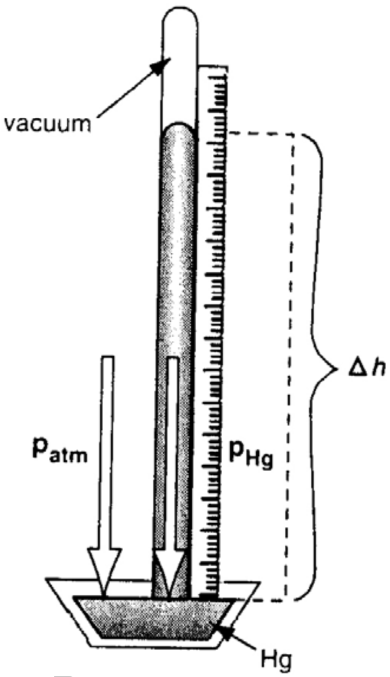
Open-end manometer would measure ***“relative pressure”*** (gauge pressure).

Relative → compare with something
In this case the atmospheric pressure is reference.

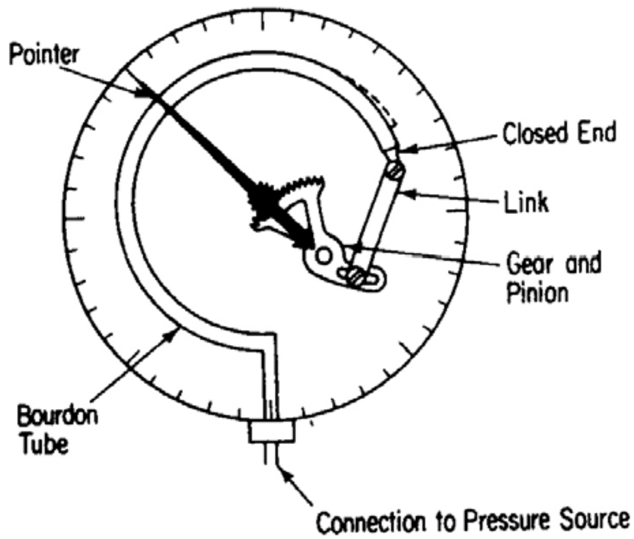
Measuring against “vacuum” or against “no pressure” → the “***absolute pressure***”

Measurement of Pressure

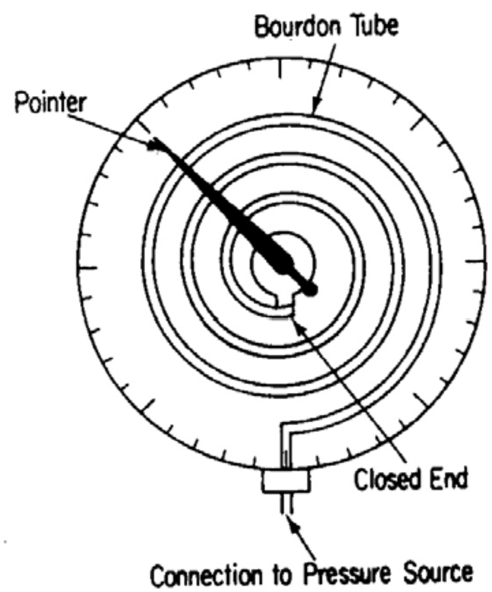
The common equipment used to measure pressure is "barometer", which is used to measure the atmospheric pressure, and "Bourdon gauge", which is use to measure the pressure.



Barometer

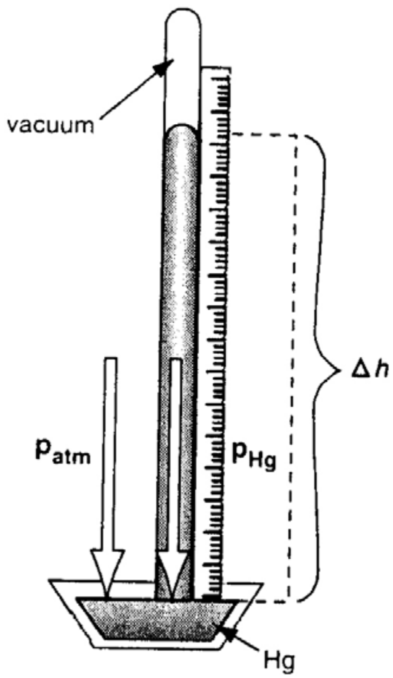


"C-type" Bourdon gauge



"Spiral-type" Bourdon gauge

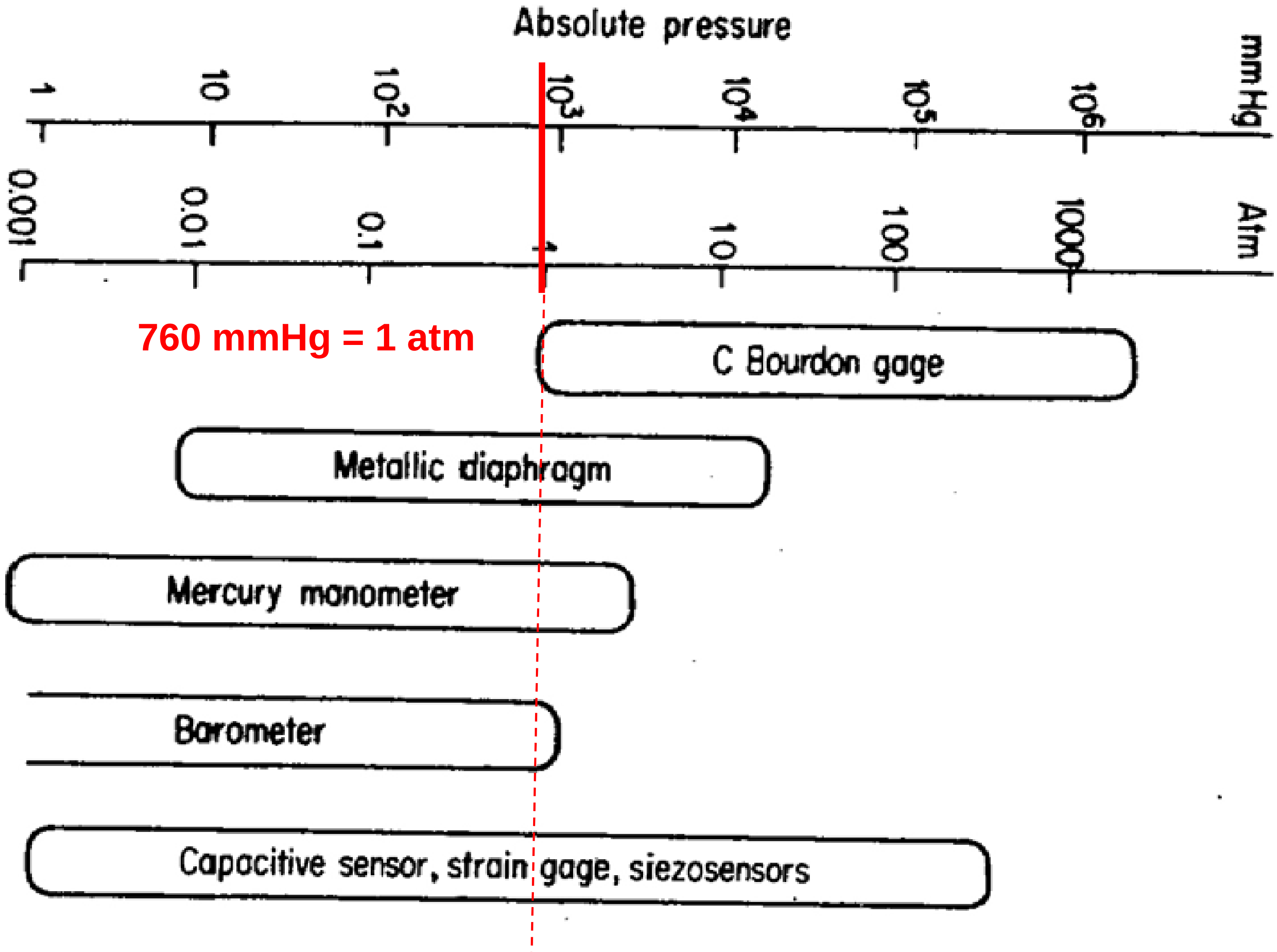
<u>HOMEWORK</u> → How these equipments could measure pressure?



"Vacuum"

Form the picture, measuring the vacuum is indicated by the scale of liquid mercury in a close-end tube, which the vacuum is achieved, e.g. inches Hg vacuum (we usually say inHg).

Thus inches Hg vacuum = barometric pressure-absolute pressure.


Absolute pressure
1
10
10^2
10^3
10^4
10^5
10^6
mm Hg
0.001
0.01
0.1
1
10
100
1000
Atm
760 mmHg = 1 atm
C Bourdon gage
Metallic diaphragm
Mercury manometer
Barometer
Capacitive sensor, strain gage, siezosensors

!!! Standard atmosphere vs Atmospheric pressure !!!

Standard atmosphere is defined as the pressure (in a standard gravitational field) equivalent to 1 atm or 760 mmHg at 0 °C or other equivalent value.

Atmospheric pressure is variable and must be obtained from a barometric measurement each time you need it.

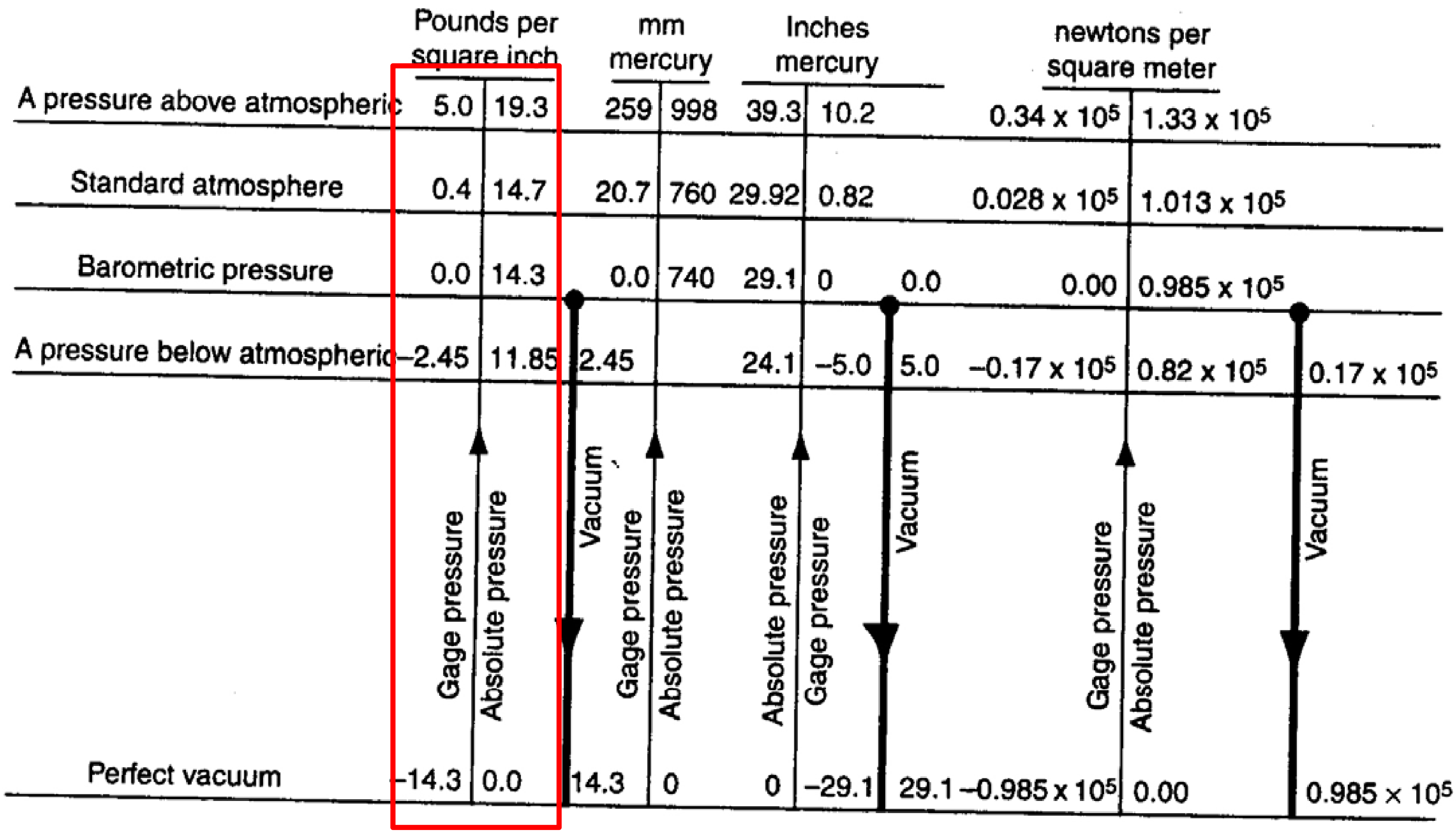
Standard atmosphere :

-1.000 atm	- 760.0 mmHg
-33.91 ft H_2O	- 1.013×10^5 Pa or N/m^2
-29.921 in. Hg	- 101.3 kPa
-14.696 psia (pounds force per square inch absolute)	

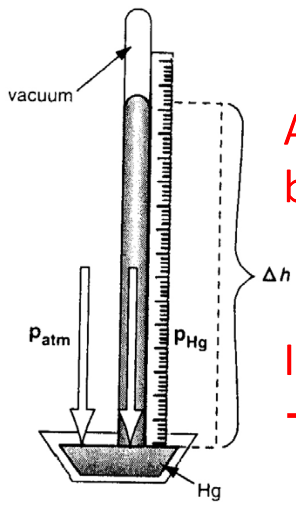
psia ang psig

psia (pound force per square inch absolute)

psig (pound force per square inch gauge) → from the measurement. Thus if you see only ***"psi"***, bear in mind that it is ***"psig"***

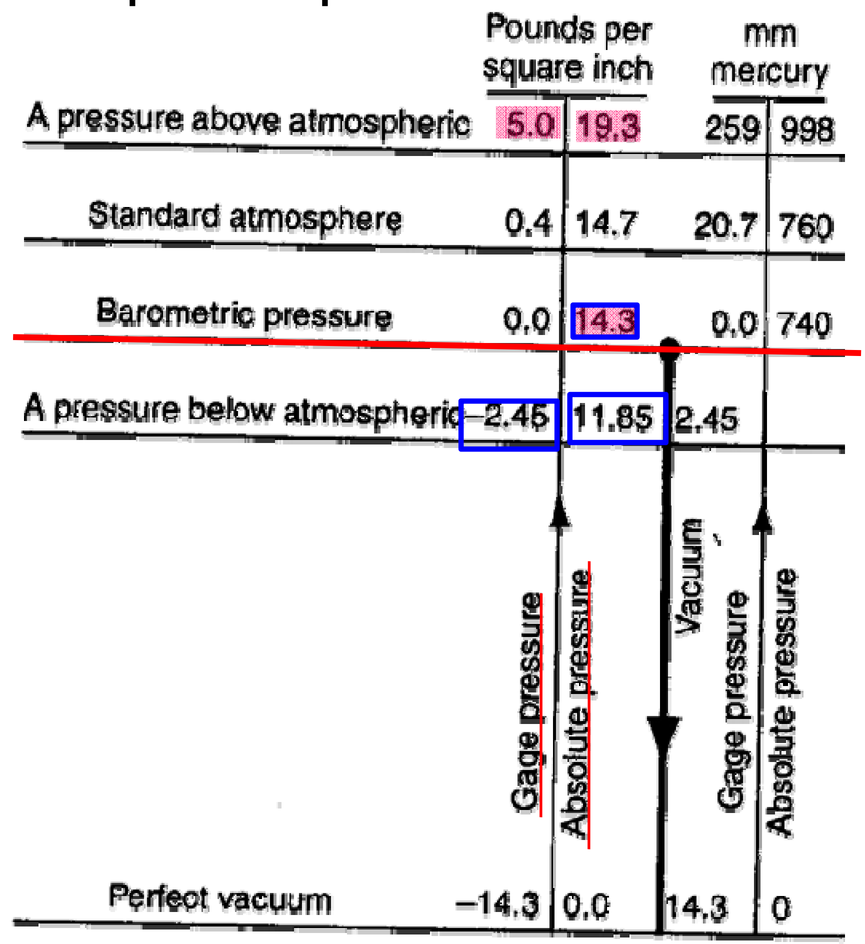


What is the relationship between atmospheric pressure/absolute pressure and gauge pressure ?



Atmospheric pressure measured by barometer = barometric pressure

Is it an absolute or gauge pressure?
→ Absolute !!!! (close-end)



<u>Pressure above atmospheric pressure</u>

Gauge pressure + Barometric pressure = Absolute pressure

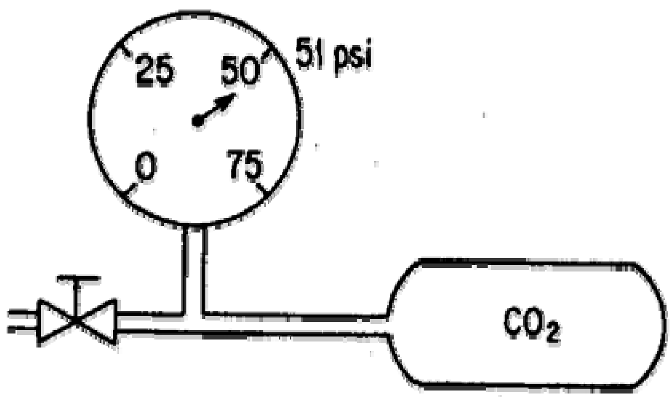
<u>Pressure below atmospheric pressure</u>

Barometric pressure – Gauge pressure = Absolute pressure

Example: The pressure gauge on a tank of CO_2 used to fill soda-water bottles reads 51.0 psi. At the same time the barometer reads 28.0 in.Hg. What is the absolute pressure in the tank in paia?

Solution:

1) What is 51.0 psi ? Is the psi = psig/psia? → **psig**
2) Barometer read 28.0 in.Hg → what is it? → **barometric pressure**
3) Draw



4) Ask for the absolute pressure, (think about the relationship)

5) Do the calculation

Gauge pressure + Barometric pressure = Absolute pressure

- Convert barometric pressure to psi

$$\text{Atmospheric pressure} = \frac{28.0 \text{ in. Hg}}{} \left| \frac{14.7 \text{ psia}}{29.92 \text{ in Hg}} \right. = 13.76 \text{ psia}$$

- Then absolute pressure = 13.76 + 51.0

= 64.8 psia ANS

!!!!! Bear in mind that you should always state the ***"absolute"*** or ***"gauge"*** of other pressure units,

e.g. 12.5 kPa absolute

32.0 mmHg absolute

760 cmHg gauge

Differential pressure measurement

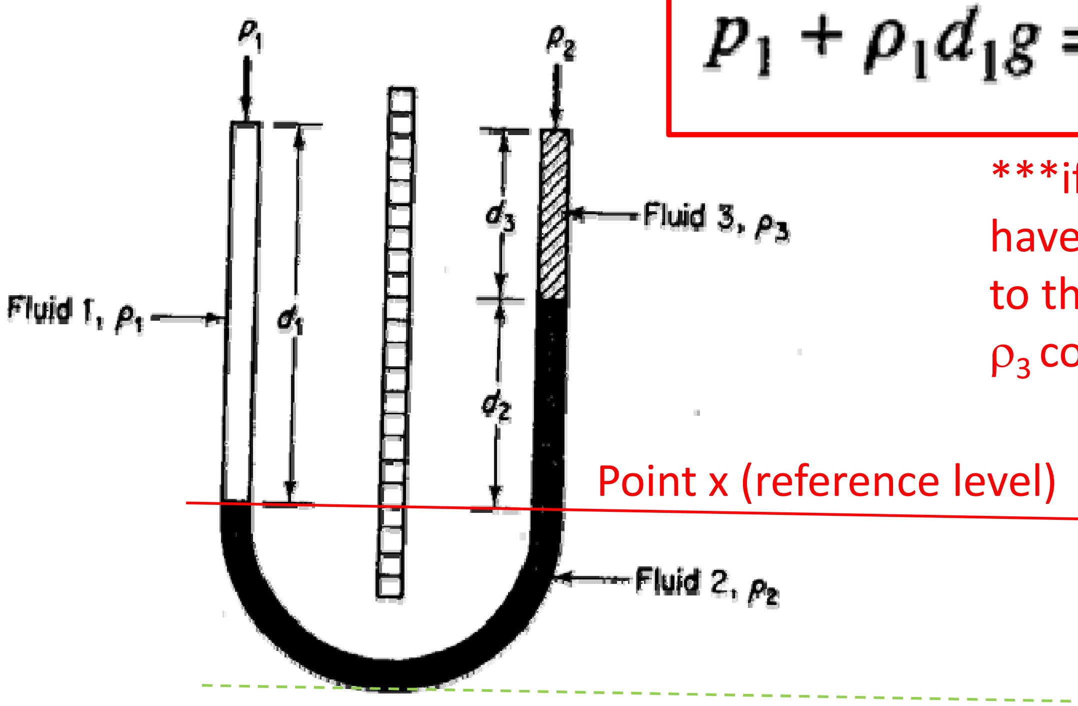
There is a relationship between pressure, density of fluids and the height of fluids in the U-tube as shows in the picture.

The lefthand and righthand of the tube must have the same pressure.

The reference level must be mentioned, if we assign point x as a reference we will get →

$$p_1 + \rho_1 d_1 g = p_2 + \rho_2 g d_2 + \rho_3 g d_3$$

***if fluid 1 and 3 are gases, which have a massive difference in ρ compare to the fluid 2, the terms involved ρ_1 and ρ_3 could be ignored.



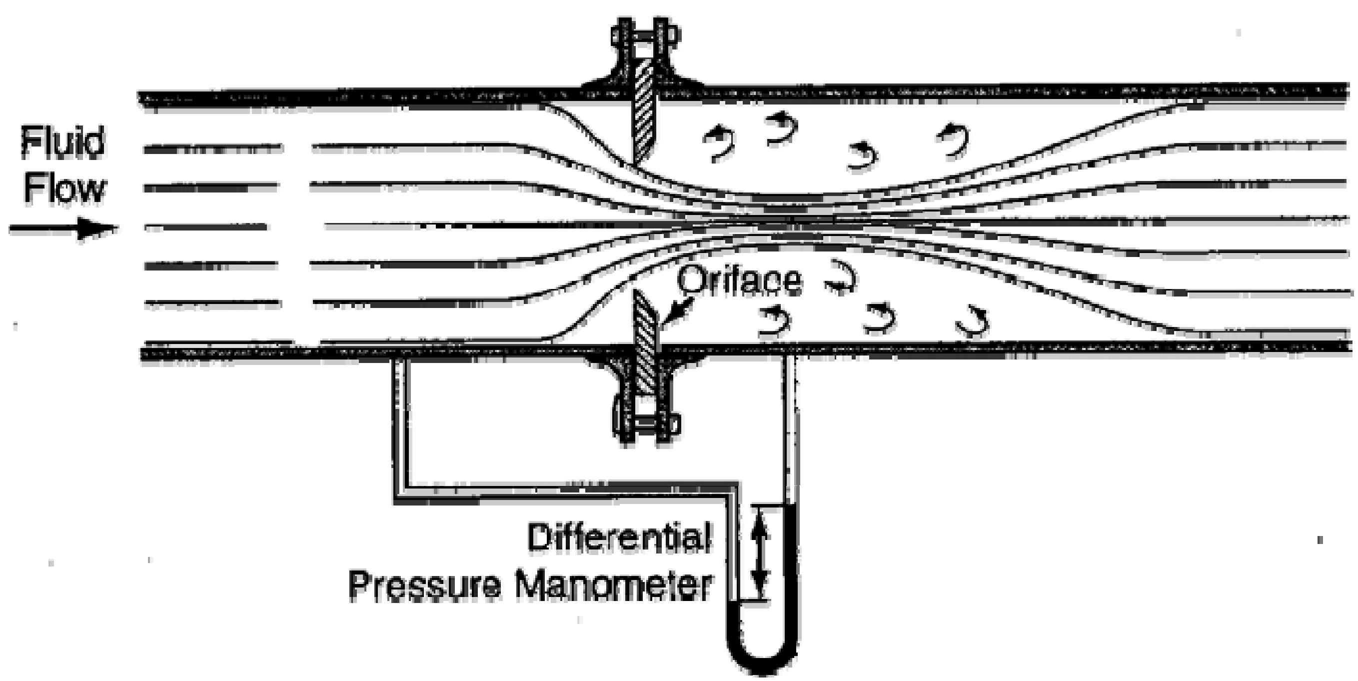
What will happen?

Differential pressure measurement

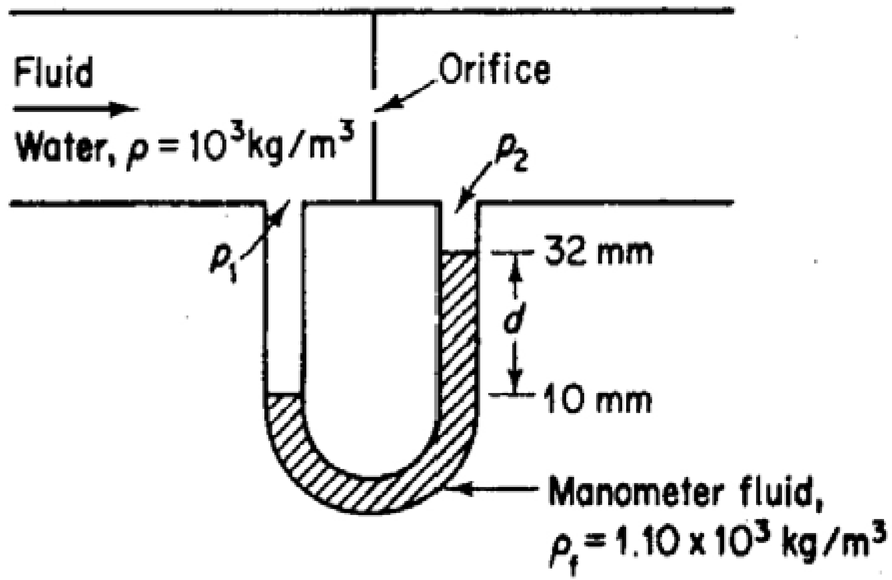
From last slide, the principle could be applied to the pipe system in order to measure the pressure difference in the pipe, where ρ_1 and ρ_3 are equal. The new equation is achieved.

$$p_1 - p_2 = (\rho_2 - \rho)gd_2$$

(p_1-p_2) is sometimes called ***"pressure drop"***.



Example: calculate the pressure drop (p_1-p_2) in pascals for manometer reading in picture below;



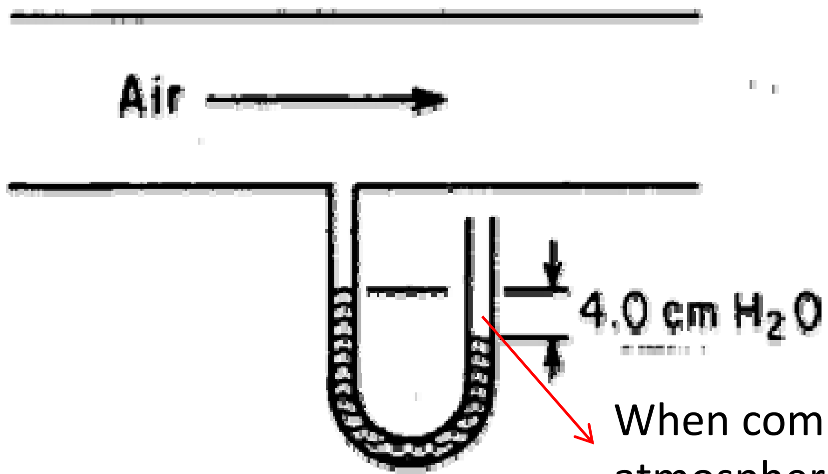
Solution:

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

$$= \frac{(1.10 - 1.00)10^3 \text{ kg}}{\text{m}^3} \left| \frac{9.807 \text{ m}}{\text{s}^2} \right| \frac{(22)(10^{-3})\text{m}}{} \left| \frac{1(\text{N})(\text{s}^2)}{(\text{kg})(\text{m})} \right| \frac{1(\text{Pa})(\text{m}^2)}{1(\text{N})}$$

$$= 21.6 \text{ Pa}$$

Example: Air is flowing through a duct under a draft of 4.0 cm H2O. The barometer indicates that the atmospheric pressure is 730 mm Hg. What is the absolute pressure of the air in inches of mercury?



When compare to air flow and atmospheric pressure, the pressure is "under atmospheric".

Solution

$$\text{Atmospheric pressure} = \frac{730 \text{ mm Hg}}{} \left| \frac{29.92 \text{ in. Hg}}{760 \text{ mm Hg}} \right. = 28.7 \text{ in. Hg}$$

then

$$\frac{4.0 \text{ cm } H_2O}{} \left| \frac{1 \text{ in.}}{2.54 \text{ cm}} \right| \frac{1 \text{ ft}}{12 \text{ in.}} \left| \frac{29.92 \text{ in. Hg}}{33.91 \text{ ft } H_2O} \right. = 0.12 \text{ in. Hg}$$

Thus absolute pressure = barometric pressure – gauge pressure
= 28.7 – 0.12 = 28.6 in.Hg. **absolute**

Home Work

Convert a pressure of 800 mm Hg to

1) psia (15.5)
2) atm (1.052)
3) kPa (106.6)
4) ft H_2O (35.6)

Page 119 in Himmelblau and Riggs Text book

*	5.3
*	5.4
*	5.13
*	5.16
**	5.23
**	5.26
***	5.34