

Principle 1 Summary

2022 / 2023

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Chapter "2" Introduction to Engineering Calculations

Chemical Engineering

raw material $\xrightarrow{\text{processes}}$ product

- * amount and properties of the raw material
- * amount and properties of the product

Units & dimensions

dimension $\left[\begin{array}{l} \text{numerical value} \\ \text{unit} \end{array} \right.$

Calculated

Volume
density
velocity

measured

mass
time
length
temperature

Force & weight

natural force unit $\left\{ \begin{array}{l} \text{SI unit } \text{Kg} \cdot \text{m/s}^2 = 1 \text{ newton} \\ \text{CGS unit } \text{g} \cdot \text{cm/s}^2 = 1 \text{ dyne} \\ \text{Am Eng. unit } \text{lbm} \cdot \text{ft/s}^2 = \frac{1}{32.174} \text{ lbf} \end{array} \right.$

$$\boxed{1 \text{ lbf} = 32.174 \text{ lbm} \cdot \text{ft/s}^2}$$

Estimate of Measured value:

$$\text{Sample mean } \bar{x} = \frac{\text{مجموع القيم}}{\text{عددهم}}$$

Range

$$R = x_{\max} - x_{\min}$$

variation

$$S_x^2 = \frac{1}{n-1} [(x_1 - \bar{x})^2 + (x_2 - \bar{x})^2 + \dots]$$

deviation

$$S_x = \sqrt{S_x^2}$$

pressure :- $\frac{\text{force}}{\text{Area}}$ $\frac{N}{m^2}$ $\frac{lbf}{m^2}$ $\frac{\text{dyne}}{cm^2}$

$$P = P_0 + \rho gh$$

$$P_{abs} = P_{gauge} + P_{atm}$$

Open end
gauge

differential
 Δ

sealed end
abs

Temperature

$C \& K$
 $R \& F$

الفرق بين



* density = $\frac{\text{mass}_{\text{sub}}}{\text{volume}_{\text{sub}}}$ { g/cm³, kg/m³, lbm/ft³ }

* Specific volume = $\frac{\text{volume}}{\text{mass}}$

✓ $\frac{\text{g}}{\text{cm}^3} \equiv \text{specific gravity} \rightarrow \text{kg} \times 1000$
 $\rightarrow \text{lbm } 62.43$

* G mole $\rightarrow 6.02 \times 10^{23}$ (Avogadro's number)

* X_{mass} fraction = $\frac{\text{mass of A}}{\text{total mass}}$

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

mass fraction $\xrightarrow[\& \text{table}]{\text{Basis of Calcul}}$ mole fraction.

* Average molecular weight

$$\frac{1}{M} = \sum \frac{X}{M} \quad M = yM$$

* Mass conc = $\frac{m \text{ of sub}}{V \text{ of solution}}$

* mol conc = $\frac{n \text{ of sub}}{V \text{ of solution}}$

* molarity = $\frac{\text{mol of solute}}{V \text{ solution (l)}}$



$$* 1 \text{ ft} = 12 \text{ Inch}$$

$$* 1 \text{ yd} = 3 \text{ ft}$$

$$* 1 \text{ N} = \text{Kg} \cdot \text{m/s}^2$$

$$* 1 \text{ dyne} = \text{g} \cdot \text{cm/s}^2$$

$$* 1 \text{ lbf} = 32.174 \frac{\text{lbm} \cdot \text{ft}}{\text{s}^2}$$

$$g = 9.8066 \text{ m/s}^2$$

$$= 980.66 \text{ cm/s}^2$$

$$= 32.174 \text{ ft/s}^2$$

Dimensionless groups

* Exponents $x^{(2)}$

* Transcendental ($\log, e, \sin$)

* arguments of transcendental $\sin(x)$

Interpolation estimate y between 2 points

$$\frac{y_2 - y_1}{x_2 - x_1} = \frac{y - y_1}{x - x_1} \rightarrow (x_2 - x_1)(y - y_1) = (y_2 - y_1)(x - x_1)$$

$$y = y_1 + \frac{x - x_1}{x_2 - x_1} \text{ common } 1$$

Fitting a straight line & non linear line
(Linearization)

Least square method

$$S_x = \frac{1}{n} \sum x$$

$$S_y = \frac{1}{n} \sum y$$

$$S_{xx} = \frac{1}{n} \sum x^2$$

$$S_{xy} = \frac{1}{n} \sum xy$$

Best Line

$$a = \frac{S_{xy} - S_x S_y}{S_{xx} - (S_x)^2}$$

$$b = \frac{S_{xx} S_y - S_{xy} S_x}{S_{xx} - (S_x)^2}$$

4 sig fig

or 5 sig fig

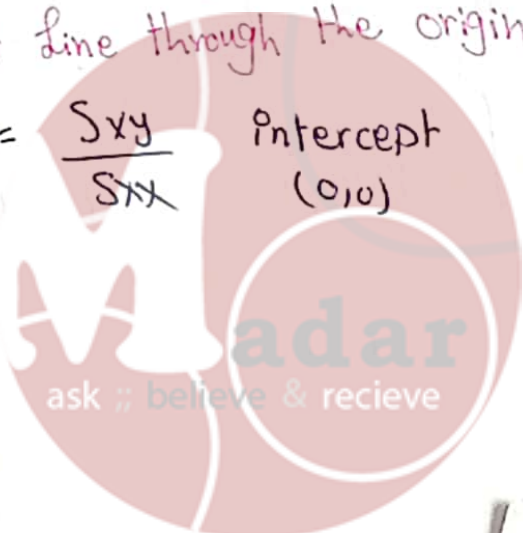
after

linearization

Best line through the origin

$$a = \frac{S_{xy}}{S_{xx}}$$

Intercept
(0,0)



Balances :- (Balance on conserved quantities (mass & energy) momentum)

① General Balance equation

Total mass $\text{input} + \overset{G}{\text{generation}} - \text{output} - \overset{C}{\text{consumption}} = \overset{A}{\text{accumulation}}$
(+) accumulation
(-) depletion

non reactive total mass $\text{input} - \text{output} = \text{accumulation}$
 $G=0 \quad C=0$

Steady state total mass $\text{input} + \text{generation} - \text{output} - \text{consumption} = 0$
 $A=0$

Total mass non reactive & steady state $\text{input} = \text{output}$

② Balance on continuous steady state process

$\text{input} + \text{generation} - \text{output} - \text{consumption} = 0$
 $A=0$

③ Balance on batch process

$\text{Initial input} + \text{generation} = \text{final output} + \text{consumption}$

Material Balance & Calculations.

* The number of independent equations $\ominus$ number of chemical species

* labiling

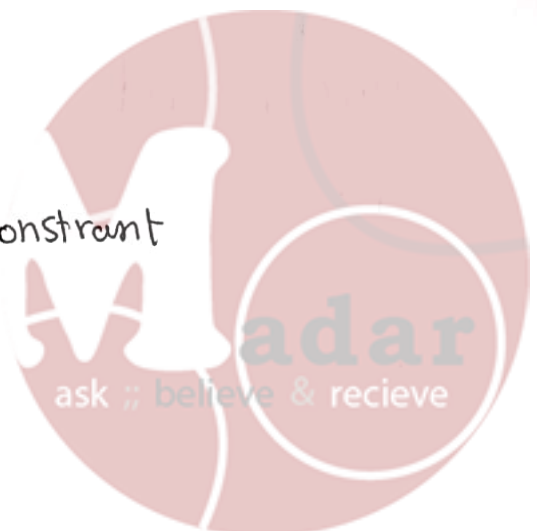
* أكتبى مطلوب السؤال بالمتغيرات

* degree of freedom

unknow
species

process constraint

$\text{Dof} = \text{Unknown} - \text{index}$



Material Balances:

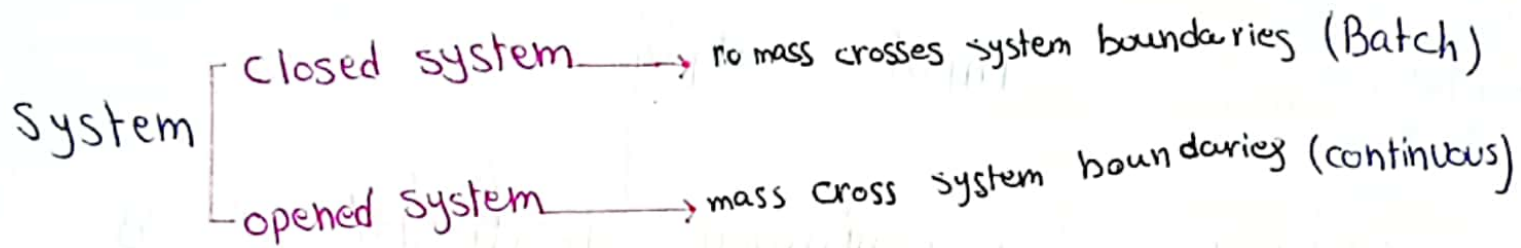
* مبدأ حفظ الكتلة :

الكتلة في نظام مغلق تبقى ثابتة مع ما حدث داخل النظام
mass can't be created or destroyed

$$\text{Total mass input} = \text{Total mass output}$$

* When do I say that my system is complete ??

- ① input & output of the entire process
- ② each individual unit satisfy Balance equation.



Chemical processes:-

Batch	Semibatch	Continuous	Steady state	transient
* كل مرة feed وحدة * كل مرة prod وحدة زي فنجرة الفلفل * Baking cake	any process that is neither batch nor continuous	input & output flow continuously	all the variables in a process don't change with time * Temp * pressure * volume * flow rate	If any of variables change with time * Batch * semi batch

↑ continuous ↓

ي يدخل نفس rate أي يطبخ عشان هيك
ما بيغير تغير

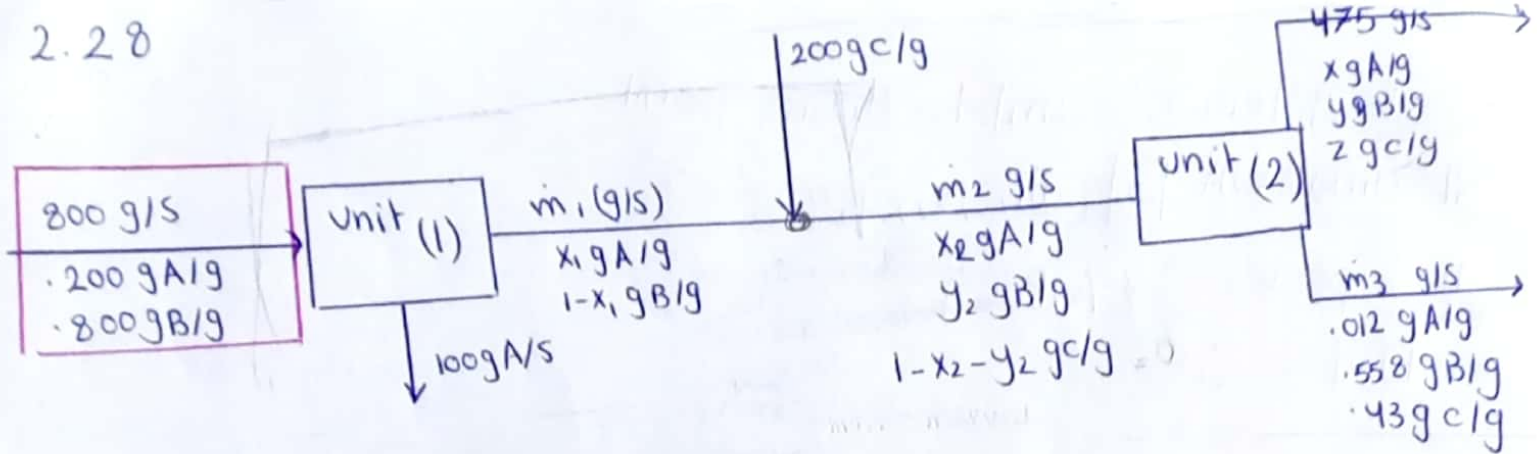
Types of balances

Differential
rate
continuous

Integral
amount
batch

ask :: believe & recieve

2.28



Step (1) Choose a Basis of calculation

Step (2) Draw a flowchart and fill all known variables & label unknown stream variables

Step (3) Express what the problem statement ask

Step (4) if you are given mixed mass and mole units for a Stream, convert all quantities to one basis (mole $\leftrightarrow$ mass)

Step (5) Do Dof analysis $Dof = 0$ ← System is balanced

subSystem "1": unit 1 ✓

unknowns = 2 { m_1, x_1 }

species = 2 { A, B }

Dof = 0

subSystem "2": unit 2

unknowns = 7 { $x_2, y_2, m_2, x_1, y, z, m_3$ }

species = 3 { A, B, C }

physical constraints = 1

Dof = 7 - 3 - 1 = 3

Sub system "3": mixing point

unknowns = 5 { m_1, x_1, m_2, x_2, y_2 }

Species: 3 { A, B, C }

Dof = 5 - 3 = 2

Sub system "4": Overall process ✓

unknowns: 4 { x, y, z, m_3 }

Species: 3 { A, B, C }

physical constraints: 1

Dof = 4 - 3 - 1 = 0

ask :: believe & recieve

Subsystem "5": unit 1 + Mixing point

unknown: $\boxed{3} \{ \dot{m}_2, x_2, y_2 \}$

species: $3 \{ A, B, C \}$

$$\text{Dof} = 3 - 3 = 0$$

Subsystem "6": unit 2 + Mixing point

unknowns: $\boxed{6} \{ \dot{m}_1, x_1, y_1, z_1, \dot{m}_3 \}$

species: $3 \{ A, B, C \}$

physical constraints: 1

$$\text{Dof} = 6 - 3 - 1 = 2$$

Step '6' write the equations in an efficient order

(minimizing simultaneous equations)

Start with system that has [Dof=0]

* unit 1

* overall process

* unit 1 + Mixing point



Just valid for mols

ملاحظات

Balances on Reactive Processes

more favorable

Molecular Species Balances	Atomic Species Balances	Extent of Reaction
No. degrees of freedom (DOF) = + No. Unknowns + No. independent Chemical reactions - No. independent Molecular species - No. process information	No. degrees of freedom (DOF) = No. Unknowns - No. independent Atomic species - No. independent Nonreactive (inert) species - No. process information	No. degrees of freedom (DOF) = No. Unknowns + No. independent Chemical reactions - No. independent Reactive species - No. independent Nonreactive (inert) species - No. process information

- * Best for single reaction
- * Need stoichiometric equation
- * Best choice when have multiple reactions
- * Most robust
- * Don't need to know the reaction is some cases
- * Convenient for chemical equilibrium problems
- * Good when equation-solving software to be used

Input + generation = output + consumption

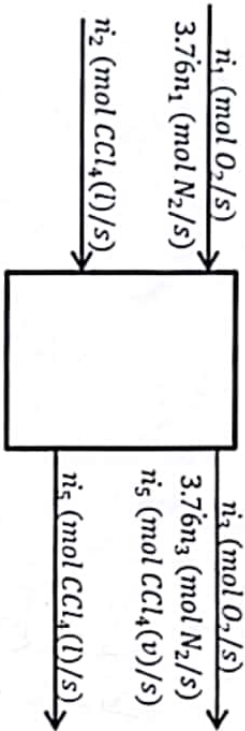
Input = output

در من السائل

$n_i = (n_i)_0 + \sum \nu_i B$

Maximum reactions

- * If 2 molecular species are in the same ratio to each other wherever they appear in a process, balances on these species will not be independent equations. Example:



- * N_2 and O_2 appear in the same ratio, 3.76 mol N_2 /mol O_2 , they cannot be counted as 2 independent molecular species; (you can write a balance on either N_2 or O_2)
- * Atomic C and Cl are always in the ratio of 1:4, so they are not independent atomic species; (you can write a balance on either C or Cl)

- * If the stoichiometric ratio of a reaction can be obtained by adding/subtracting multiples of other equations, it is not independent chemical reaction. Example:

- [1] $A \rightarrow 2B$
- [2] $B \rightarrow C$
- [3] $A \rightarrow 2C$

Now, [3] = [1] + 2*[2] $\rightarrow$ it's not independent $\rightarrow$ those 3 reactions have only 2 independent chemical reactions.

Chapter 5: Single phase system

In the system only one phase
(solid or liquid or gas)

Ss 5.1: Liquid & Solid densities:

* Solids & liquids densities are independent of Temperature & pressure.

* mixture of pure components

$$\bar{P} = \sum X_i P_i \quad \sum \frac{1}{\bar{P}} = \sum \frac{X_i}{P_i} \quad (\text{volum additivity})$$

* $\dot{V}(STP) \rightarrow \dot{n}$ ليست للتعبير عن $\dot{V}$ وإنما طريقة أخرى للتعبير عن $\dot{n}$

IDEAL GASES

(depends on T & P)

$$PV = nRT \rightarrow \bar{P} = \frac{P\bar{M}}{RT} \quad \bar{M} = \sum X_i M_i \quad \text{mixture of gases}$$

assumption:

① negligible volume

② exert no forces on each other

③ Collide elastically with the walls of container

Conditions:

high T ↑ low pressure P ↓

make sure that it IDEAL GAS??

$$\frac{V}{n} = \frac{RT}{P} \quad \begin{cases} \text{diatomic} > 5 \text{ L/mol} \\ \text{other} > 20 \text{ L/mol} \end{cases}$$

same gas different conditions

$$\frac{PV}{P_s V_s} = n \frac{T}{T_s}$$

Dalton's law $P_A = y_A P$

Amagat's law $V_A = y_A V$

volum fraction of a substance in an ideal gas mix = mol fraction of this sub

Non IDEAL GASES

Verial equation of state:

$$\frac{P\hat{V}}{RT} = 1 + \frac{B}{\hat{V}} \quad (\text{not for polar compounds})$$

$P \rightarrow$ straight forward

$\hat{V} \rightarrow$ quadratic equation

Refer to book!

Van der waals equation of state:

$$P = \frac{RT}{\hat{V}-b} - \frac{a}{\hat{V}^2} \quad \begin{matrix} \text{He \& H}_2 \\ + 8 \text{ K} \\ + 8 \text{ atm} \end{matrix}$$

same - Redlich SRK

$$P = \frac{RT}{\hat{V}-b} - \frac{a\alpha}{\hat{V}(\hat{V}+b)}$$

Compressibility factor

$$Z = \frac{P\hat{V}}{RT} \quad V_r^{\text{ideal}} = \frac{\hat{V}}{V_c} = \frac{P_c \hat{V}}{R T_c}$$

Mixture of gases (Kay's rule)

$$T_c = y_A T_{cA} + y_B T_{cB} \quad T_r = T/T_c$$

$$P_c = y_A P_{cA} + y_B P_{cB} \quad P_r = P/P_c$$

$$\hat{V} = \sum z_m R T$$

* Batch process v is constant

* Complete reaction is one where all of (irreversible) at least one of available reactants is used up to converted into products (when it reached equilibrium) reversible

* fractional conversion normally for L.R except if he says something else.

* hydrogenation is reversible

* Combustion complete لا تخلص بغير complete

* $\dot{V}$ STP $\dot{n}$ طريقة أخرى للتعبير عن

* $\underline{\underline{\dot{V}}}$ Volumetric flow rate $\underline{\underline{\dot{V}}} = \frac{\dot{V}}{n}$ منها يقدر اطلع عدد المولات

* V_r $\underline{\underline{I}}$ دينا نطلع قيمة (Z) مستخدم V_r ما يكون هو معيناً

$$V_r = \frac{P_c \hat{V}}{R T_c}$$



Chapter "6" :- MULTIPHASE SYSTEM

phase change operations :-

* freezing * melting * evaporation * condensation

separation & purification processes :-

* leaching * absorption * Distillation

* adsorption * crystallization * liquid extraction.

difference between evaporation & boiling

evaporation (surface) $\rightarrow p^* < p \rightarrow$ Total pressure

boiling (entire liquid) $\rightarrow p^* = p$

difference between Saturation & humidity

saturation gas-vapor

humidity air-water

* Vapor pressure $\rightarrow$ liquid-gas equilibrium curve

* number of mols cond = number of mol in gas if it completely cond

* Humidity :- water vapor that's in the air

* relative humidity = $\frac{p_{H_2O}}{p^*(H_2O)} \times 100\%$ (dependent on T)

$p_{H_2O} \rightarrow$ gives an idea of the amount of H_2O in the air

$p^*_{H_2O} \rightarrow$ maximum amount of water that can be in the air at a given (T)

* absolute humidity = $\frac{\text{mass of } H_2O \text{ in the air}}{\text{mass of dry air}}$

* molal humidity = $\frac{\text{mol of } H_2O \text{ in air}}{\text{mol of dry air}}$

Single Component phase equilibrium

* Volatility :- species tends to transfer from liquid (solid) to vapor

Volatility $\uparrow$ $\rightarrow$ vapor
Volatility $\downarrow$ $\rightarrow$ condensed form (liquid or solid)

* Vapor pressure :- P^*
* measure its volatility
* vapor liquid equilibrium curve
Vapor pressure $\uparrow$ volatility $\uparrow$

① Clausius - Clapeyron equation

$$\ln P^* = -\frac{\Delta H_v}{RT} + B \quad \left[\ln P^* \text{ vs } \frac{1}{T} \right]$$

(heat of vaporization)

② Cox chart

③ Antoine equation

$$\log P^* = A - \frac{B}{(C/T) + C}$$

④ Interpolation

$$y = y_1 + \frac{x - x_1}{x_2 - x_1} (y_2 - y_1)$$

GIBBS phase equilibrium

Def multiple phase system

Intensive variables at equilibrium if there is no reaction

$$DF = 2 + C - \pi$$

number of phases in the system

Chemical species

equilibrium state :-

- * Temperatures & pressures of both phases are the same
- * The composition of each phase no longer change to describe the system :-
- ① Temperature & pressure
- ② masses of each phase
- ③ mass or mol fraction for each phase

Gas - Liquid system

One Condensable component

(sm, sc, sr sp)
Saturated: Solution holds all material that it can hold at the system Temperature & pressure.

$$P_i^*(T) = y_i P = P_i^o$$

Valid: ① saturated
② only one species that can condense (condensable)

* gas in equilibrium liquid is saturated with volatile component
* partial pressure of vapor at equilibrium can't exceed the vapor pressure of pure component

- * Super heated $P_i = y_i P < P_i^o$
- * dew point :- $P_i = y_i P = P_i^o$
The temperature at which the vapor becomes saturated
- * degrees of superheat difference between the system Tem & dew point of gas

MULTI Component

Gas - Liquid Systems
* Composition of components in 2 phases are not independent
IDEAL SOLUTIONS
Raoult's law

$$y_i P = x_i P^*_{\text{liquid}}$$

- * x_i nearly 1
- * mixture of similar subs

Henry's law

$$y_i P = x_i P_i^o(T)$$

- * x_i nearly 0
- * non condensable gases

Bubble point temperature
liquid heated slowly at const P $\times$ liquid form
 $P = x_A P^*(T_P) + x_B P^*(T_P)$
gas $y_i = P_i / P$

dew point temperature
gas cooled $\rightarrow$ first liquid droplet
 $P_{DP} = \frac{y_1 P^*_{\text{top}} + y_2 P^*_{\text{top}}}{P_i / P_{DP}}$
 $x_i = \frac{y_i P^*_{\text{top}}}{P_i / P_{DP}}$