CHEMICAL ENGINEERING PRINCIPLES I

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Units and Dimensions

measured : Length , time , mass , temperature

calculated by × or ÷ other dimensions : . velocity = Length/time

. volume = $(\text{Length})^3$. Density = mass/$(\text{Length})^3$

SI and american engineering system units :

	SI	CGS	Am. Eng. unit
Mass	Kg	g	pound (lbm)
Length	m	cm	ft
Time	S	S	S
Temperature	K	K	Rankine (°R)
Mole	gram mole (g-mol)	gram mole (g-mol)	pound mole (lb-mole)

Conversion factor :

$$\text{New unit} = \text{old unit} \left(\frac{\text{new unit}}{\text{old unit}}\right)$$

$$\frac{1}{\text{new}} = \frac{1}{\text{old}} \left(\frac{\text{old}}{\text{new}}\right)$$

force is propotional to the product of mass and acceleration

$1\ N = 1\ kg \cdot m/s^2$ SI

$1\ dyne = g \cdot cm/s^2$ CGS

$1\ lbf \doteq lbm \cdot ft/s^2$ American engineering

↳ pound force

$1\ lbf = 32.174\ lbm \cdot ft/s^2$

Gravitational acceleration (g) varies directly with the mass, inversly with the squar of distance.

Example on calculating weight: (الوزن)

$m = 124\ lbm$ $w = ?$

$g = 32.174\ ft/s^2$ $w = m \times g$

$= 124\ lbm \times 32.174\ ft/s^2$

$w = 3989.6\ lbm \cdot ft/s^2$

$1\ lbf = 32.174\ lbm \cdot ft/s^2$

$? \times = 3989.6\ lbm \cdot ft/s^2$

$w = 124\ lbf$

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Significant figures:

number of digits starting from left and from the first non zero. ⟶

- If there's decimal point: from the first non zero digit on the left to the last digit (zero or non zero)

  0.04600 (4 sig. fig)

- No decimal points: From the first non zero (on the left) to the last non zero.

  23040 (4 sig fig)

* Multiplication and division.

The sig. fig in the answer should be the smallest number of sig. fig in the equation that's multiplied or divided.

Example: 279 × 83 = 23,157 ⟶ 23000

3 sig fig (2 sig fig)

more sig figs ⟶ more precise

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* Addition and subtraction

Example: $4.231 + 3.51 = 7.741 = 7.74$

Last digit of sig fig

$420. + 3.51 = 423.51 = 424$

3 sig fig, 3 sig fig

$300 - 47.465 = 252.535 = 300$

non sig

Remember: عند التقريب وكان الرقم 5 ، لازم يكون الجواب رقم زوجي .

$1.55 \simeq 1.6$

$1.45 \simeq 1.4$

in scientific notation

$5.4 \times 10^3 + 2.1 \times 10^4$

$0.\underset{2\ sig}{54} \times 10^4 + \underset{2\ sig}{2.1} \times 10^4$

$= 2.6 \times 10^4$

(2) (1)

$(2.1 \times 10^3)(4 \times 10^5)$

$(2.1 \times 4)\ (10^3 \cdot 10^5)$

$8.4 \times 10^8 \simeq 8 \times 10^8$

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More sig. figs → more precision

How to find the ranges within a value?

- 8.3 $8.3 + 0.05 = 8.35$ $8.3 - 0.05 = 8.25$

$\frac{\text{جزء من خزة } (0.1)}{2}$ $= \pm 0.05$

"value lies between 8.25 and 8.35"

2. تقسيم sig fig على last digit بدون أرقام

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Checking an arithmetic (حسابية) calculations :

1. Use scientific notation for very small and large numbers.

2. Do the calculations by hand (بدون آلة حاسبة), rounding numbers

3. drop the small number when added to a large number.

• أهم نقطة في التفكير اذا الجواب منطقي ؟

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Why we don't get the same value in each run ? "عدم تكرار النتيجة عند اعادة التجربة"

1. Change in temperature from one run to another.
2. Difference in time.
3. variations in sampling (اختلاف في اخذ العينات)

How to estimate the true value ?

By the sample mean.

Sample mean : $\bar{x} = \frac{x_1 + x_2 + \cdots x_N}{N}$

• كلما زاد عدد مرات اجراء التجربة ، كانت estimated value لـ x افضل ، الا اذا كان هناك خطأ في اجراءات التجربة أو بالجهاز .

Range : $R = x_{max} - x_{min}$

Sample variance : $S_x^2 = \frac{(x_1 - \bar{x})^2 + (x_2 - \bar{x})^2 + \cdots}{N - 1}$

Sample Standard deviation: $S_x = \sqrt{S_x^2}$

• كلما قل Range كانت القراءة أدق ، ولكن هناك طرق أفضل لمعرفة اي القراءات أدق وسوف يعد ما عن الـ mean :

• S_x^2

• S_x [S_x^2 or S_x تكون القراءة ادق اذا كان أقل .]

value of measured value (x)

$x = \bar{x} \pm$ error

↳ mean value of the data.

error: Range $x_{max} - x_{min}$ or

S_x , $2S_x$, $3S_x$

Test your self p: 19

a. $\bar{x} = \frac{232 + 248 + \dots}{5} = 237.4 \ cm^3/s$

Range: $248 - 227 = 21 \ cm^3/s$

$Sx^2 : \frac{(232 - 237.4)^2 + (248 - 237.4)^2 + \dots}{5-1} = 66.3 \ cm^6/s^2$

$Sx = \sqrt{66.3} = 8.1 \ cm^3/s$

b. $V = a \pm b$ "within 2 Sx"

$(237. \pm 16.2)$ a = mean $b = 2\,Sx$

$= 2 \times 8.1$

$= 16.2$

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2.6 Dimensional Homogeneity.

. dimensions لازم تكون الي نفس ال valid equation ي!

Ex:

$$V\ (m/s) = V_i\ (m/s) + g\ (m/s^2)\ t\ (s)$$

- Every valid equation must be dimensionally homogeneous.
- An equation may be dimensionally homogeneous and invalid (غير صحيح)

Ex: $V\ (m/s) = V_i\ (m/s)$

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Dimensionless quantity :

- pure number (2, 1.5, 4/3)
- Dimensionless group (M/M_0)
- Exponents "z" in $\rightarrow$ (x^z)
- Transcendental functions (Log, exp = e) and Sin

Test your self p: 22

1. All terms must have the same dimensions, NO, YES.

2. $a\,(m/s^2) = a\,z\,(m^3)$ $\quad a = ?$

$$\frac{\text{acceleration}}{\text{volume}} = \frac{a \cancel{\text{volume}}}{\cancel{\text{volume}}} \qquad a = \frac{m}{s^2} \times \frac{1}{m^3} = m^{-2} \cdot s^{-2}$$

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3. Combination of factors with no net units.

$r(m)$, $S(m/s^2)$, $t(s)$ = 1 ?

$$m \cdot \frac{s^2}{m} \times \frac{1}{s^2} \longrightarrow \frac{r}{s \cdot t^2}$$

4. $z(lbf) = a \sin(Q)$ a and Q ?

Force = a

a (lbf) ✓ , Q is dimensionless

becuase of (sin)

2.7 process data representation and analysis

when I can't measure a variable directly , we measure another related one.

Interpolation

- Inside the range.
- when data are near to eachother and linear relationships

(علاقة خطية)

Extrapolation

- out side the range
- Also for linear relation,
- If we use it on a curve it will cause a huge error.

زختار نقطتين قرايب من بعض

(اذا كان Curve).

Equation of the line through (x_1, y_1) and (x_2, y_2):

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

Test your self p: 23

1. a. $f \rightarrow y$

$t \rightarrow x = 1.3$

(between $t=1$ and $t=2$)

$$y = 1 + \frac{1.3 - 1}{2 - 1}(4 - 1) = 1.9$$

b. $t \rightarrow y$ $\quad f \rightarrow x = 5$

(between $f=4$ and $f=8$)

$$y = 2 + \frac{5 - 4}{8 - 4}(3 - 2) = 2.25$$

Fitting a straight Line :

$$y = ax + b$$

- $y = 3x + 4$ (plot y versus x)
- $y = 4.24 (x-3)^2 - 23$ (plot y versus $(x-3)^2$)
- $y = \dfrac{1.3 \times 10^7 \sin(2x)}{x^{1/2} + 58.4}$

$$1/y = \frac{x^{1/2} + 58.4}{1.3 \times 10^7 \sin(2x)} \longrightarrow \frac{\sin(2x)}{y} = \frac{x^{1/2} + 58.4}{1.3 \times 10^7}$$

(plot $\dfrac{\sin 2x}{y}$ versus $x^{1/2}$) $a = 1/1.3 \times 10^7$

$b = 58.4 / 1.3 \times 10^7$

Fitting non Linear data:

(Quantity 1) = a (Quantity 2) + b

$\sin y = a(x^2 - 4)$ plot $\sin y$ versus $(x^2 - 4)$

Line through the data must be zero ? because

$b = 0$ no intercept

$y = 1 + x(mx^2 + n)^{1/2} \longrightarrow y - 1 = x(mx^2 + n)^{1/2}$

$\left(\dfrac{y-1}{x}\right)^2 = mx^2 + n$ plot $(y - 1/x)^2$ versus x^2

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Test yourself p: 27

1. $y = a(x^2 - 2)$

2.

a. plot y versus $\sqrt{x}$ $\quad a = \dfrac{y_2 - y_1}{\sqrt{x_2} - \sqrt{x_1}}$ $\quad b = y_1 - a\sqrt{x_1}$

b. plot $1/y$ versus $(x-3)^2$ $\quad a =$ slop $\quad b =$ intercept

c. $(y)^3 = (ax^2 - b)^{1/3}$ $\quad$ plot y^3 versus x^2

$y^3 = ax^2 - b$ $\quad$ slop $= a$ $\quad$ intercept $= -b$

d. $1/\sin y = \dfrac{(ax+b)^2}{x}$

$x/\sin y = (ax+b)^2$

$\sqrt{x/\sin y} = ax + b$ $\quad$ plot $\sqrt{x/\sin y}$ versus x

slop $= a$ $\quad$ intercept $= b$

e. $\ln y = \ln a + bx$

plot $\ln y$ versus x

slope: $b = \dfrac{\ln(y_2/y_1)}{x_2 - x_1}$ $\quad$ intercept $\quad \ln a = \ln y_1 - bx_1$

f. $\ln y = \ln a + b \ln x$ $\quad$ plot $\ln y$ versus $\ln x$

slope $b = \dfrac{\ln(y_2/y_1)}{\ln(x_2/x_1)}$

intercept $\quad \ln a = \ln y_1 - b \ln x_1$

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CH 3 : process and process variables

- process: any operation or a series of operations by which a particular object is accomplished.
- chemical process: any operation or a series of operations by which a particular product is produced from raw materials.
- process variables: temperature - pressure - mass flow - volumetric flow and chemical composition.

We have 2 types of variables :

1. Measurements to quantify a material (كمية)
   - mass, volume, mole.

2. Measurements to specify process conditions.
   - pressure, temperature.

- The material that enters a process → Input or feed
- The material that leaves a process → Output or product

process streams (نعبر عنها بشكل أسهم)

3.1 Mass and volume

Density (ρ) is used as a conversion factor between mass and volume or between mass flow rate and volumetric flow rate.

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Mass flow rate ?? (mass per time) سرعة تحرك ال

- Liquid and Solid densities vary slightly with temperature and pressure.
- Gas density depend heavily on temperature and pressure.

Specific volume: It's the inverse of density.

$= \frac{1}{\text{density}} = \frac{\text{Volume}}{\text{mass}}$

Specific gravity: The ratio of a density of a substance to the density of refrence substance at a specific condition

$(SG = \rho / \rho_{ref})$

Typical ρ_{ref} ⟶ water at 4 c° and 1 atm

$1\ g/cm^3 = 1\ kg/L = 1000\ kg/m^3 = 62.43\ lbm/ft^3$

specific gravity is given at particular temperature

(reference temperature مش شرط تكون)

To get density from (SG)

SG is given, and ρ_{ref} for water is: $1\ g/cm^3$

$1\ kg/L = 1000\ kg/m^3 = 62.43\ lbm/ft^3$

$(\rho = S.G \times \rho_{ref})$

		SG (20/4)	Tm (C°)	Tb (C°)
Methanol	CH_3OH	0.792	−97.9	64.7
water	H_2O	1.00 (4°)	0	100

SG for methanol → 0.792 (20°/4°), specific gravity of methanol at 20C° with reference to water at 4C° is 0.792.

Tm (C°) → melting point at 1 atm.

Tb (C°) → Boiling point at 1 atm.

Test your self p: 44

1. Dimensionless $SG = \rho/\rho_{ref} = g/cm^3 / g/cm^3 = 1$

2. $\rho = SG \times \rho_{ref} = 0.5 \times 1\ g/cm^3 = 0.5\ g/cm^3$

- specific volume = 1/density = 1/0.5 = 2 cm^3/g

- $0.5\ g/cm^3 \times \frac{1\ lbm}{453.593\ g} \times \left(\frac{100\ cm}{3.2808\ ft}\right)^3 = 31.2\ lbm/ft^3$

- $m = 3\ cm^3 \times 0.5\ g/cm^3 = 1.5\ g$

- $V = \frac{18\ g}{0.5\ g/cm^3} = 36\ cm^3$

3. $\rho(A) = \rho(B) = 1.34\ g/cm^3$ $\quad v(A) = v(B) = 3\ cm^3$

$m(A) \overset{?}{=} m(B)$?? $\quad \rho = m/v \Rightarrow m = 1.34 \times 3 = 4\ g$

(Yes)

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4. $SG(A) = SG(B) = 1.34$

$V(A) = V(B) = 3\ cm^3$

$m(A) \overset{?}{=} m(B)$?

$SG = \frac{\rho}{\rho_{ref}}$ → m/v

No, there could be a difference in using ρ_{ref}.

5. . Bottel of water → broke

Volume ↑ so it's density

decreased ↓.

. butyl alcohal

volume ↓ decreased because of the (concave walls)

so it's density increases ↑.

6. when increasing T, mercury expands (يتمدد)

Volume ↑, so the density decreases.

3.2 Flow rate

Rate at which a material is transported through a process line.

1. Mass flow rate $\dot{m}$ (mass / time)
2. Volumetric flow rate $\dot{V}$ (volume / time)

$\rho = \dot{m} / \dot{V}$

Test yourself p: 46

1. $\dot{m} = 6.59$ g/s $\dot{V} = \dot{m}/\rho = \frac{6.59 \text{ g/s}}{0.659 \text{ g/cm}^3} = 10 \text{ cm}^3/\text{s}$

   $\rho = 0.659$

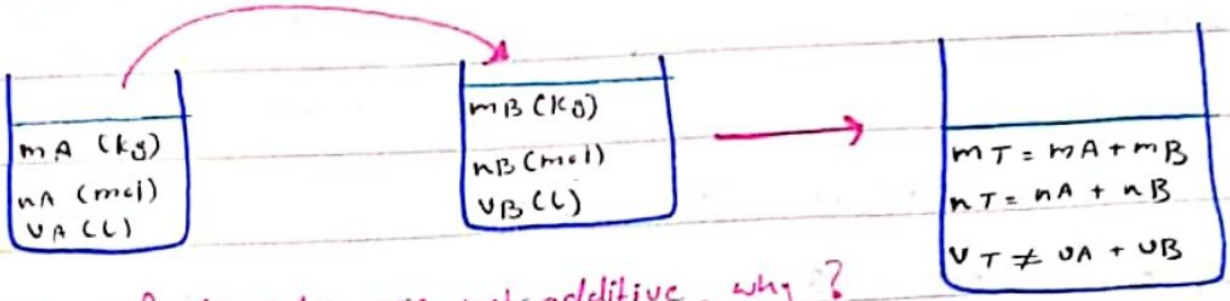
2. $\dot{V} = 100 \text{ cm}^3/\text{min}$ $\dot{m} = \rho \times \dot{V} = 1.595 \text{ g/cm}^3 \times 100 \text{ cm}^3/\text{min}$

   $\rho = 1.595 \text{ g/cm}^3$ $= 159.5 \text{ g/min}$

3. $\dot{m}_{in} = \dot{m}_{out}$

   - $\dot{V}$ doesn't change $\dot{V} = \dot{m}/\rho = \frac{\dot{m} \text{ constant}}{\rho \text{ constant}} = \dot{V}_{constant}$
   - $\dot{V}$ increases, (علاقة عكسية بين $\dot{V}$ و ρ)

Conservation of mass and volume



Volume of liquids are not additive, why ?

Because of the molecule bonding between water and the other substance, volume decreased. ↓

Test yourself p: 47

1. $t = 30$ s $v = 50$ml

   $\dot{V} = ?$ $\frac{50 \text{ mL}}{30 \text{ s}} \times \frac{60 \text{ s}}{1 \text{ min}} = 100 \text{ mL/min} = \dot{V}$

   $\dot{m} = ?$ $1 \text{ mL} = 1 \text{ g} \longrightarrow 100 \text{ g/min} = \dot{m}$

2. Devices that provides reading of the flow rate.

rotameter: خراطة سباكة orifice meter: حاب فتحة الضغط

3. density of gas is much less, so gas must flow higher than liquid.

reading would be too low.

Conversion between mass and moles

To convert number of moles to mass, using the molecular weight:

$$M.w = \frac{mass}{mole} \left(\frac{m}{w}, \frac{g}{g\,mol}, \frac{kg}{k\,mol}, \frac{Ibm}{Ib\,mol} \right)$$

M.w of water is 18, then:

1 g mol, mass = 18 g of H_2O $\longrightarrow$ Mw = 18 g / g mol

1 k mol, mass = 18 kg of H_2O $\longrightarrow$ Mw = 18 kg / k mol

Ib mol, mass = 18 Ibm of H_2O $\longrightarrow$ Mw = 18 Ibm / Ibmol

Remmember!

1 mol = 6.023×10^{23} molecules of any substance

1 k mol = 1000 mol.

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Test yourself p: 49

1. a. 1 mol = 6.02×10^{23}

b. m = n gmol x M gram/mol = M grams

2. Molecular weight of species in tons.

3. Ib moles → Ibm (mass)

2 Ibmol H → m(H) = 2 x 1 = 2 Ibm

1 Ibmol H_2 → m(H_2) = 1 x 2 = 2 Ibm

1 Ibmol O → m(O) = 1 x 16 = 16 Ibm

4. 2 kmol of C_3H_8

g mol = ? $\quad 2 \text{ kmol} \times \frac{1000 \text{ gmol}}{1 \text{ kmol}} = 2000 \text{ g mol}$

5. $\dot{m} = 100$ kg /h

$\dot{n} = ?$ $\quad$ Mw of H_2 = 2 kg /kmol

$\dot{n} = \frac{100 \text{ kg/h}}{2 \text{ kg /kmol}} = 50 \text{ kmol /h} \times \frac{1000 \text{ gmol}}{1 \text{ kmol}} = 50000 \text{ gmol}$

Mass fraction and Mole fraction

Mass fraction : $x_A = \frac{\text{mass of A}}{\text{total mass}}$ $\quad \left[\frac{\text{kg A}}{\text{kg total}}, \frac{\text{g A}}{\text{g total}}, \frac{\text{Ib}}{\text{Ibm}}\right.$

Mole fraction : $y_A = \frac{\text{moles of A}}{\text{total moles}}$ $\quad \left[\frac{\text{kmol A}}{\text{kmol total}}, \frac{\text{gmol A}}{\text{gmol total}}, \frac{\text{Ibm}}{\text{Ibm tot}}\right.$

Mass percent of A 100 x_A .

Mole percent of A 100 y_A .

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Mass is conserved.

Moles are not conserved.

Conversion from mole to mass fraction.

1. Assume 100 g mols.
2. calculate number of moles for each species.

   n = mole fraction x n_{total}. $\xrightarrow{(100)}$
3. Find M.w for each species.
4. calculate mass for each species.

   (add all masses to know the total)
5. calculat mass fraction.

Conversion from mass fraction to mole fraction.

1. Assume 100 g.
2. Calculate mass for each species.

   mass = x . m_{total} $\xrightarrow{(100\ g)}$.
3. divide by M.w to get moles. $n = m/M.w$
4. Add number of moles.
5. Calculate mole fraction.

Note: Sum of mol fraction or mass fraction must be 1.

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Average molecular weight $\bar{M}$

- $\bar{M} = y_1 M_1 + y_2 M_2 + \cdots\cdots$
- $\frac{1}{\bar{M}} = \frac{x_1}{M_1} + \frac{x_2}{M_2} + \cdots\cdots$
- $\bar{M} = \frac{m\ total}{n\ total}$

y : mole fraction
M : molecular weight
x : mass fraction

Test yourself p: 52

m.w (H) = 1 m.w (Br) = 80

1. a. $x = \frac{m\ Br}{m\ total} = \frac{80}{80+1}$

$x = 0.987$

mass = n × M.w

m (H) = 1 × 1 = 1 m(Br) = 1 × 80 = 80

b. $y = \frac{n\ Br}{n\ total} = \frac{1}{2} = 0.5$

$n\ (Br) = \frac{m}{M.w} = \frac{80}{80} = 1$

$n\ (H) = 1/1 = 1$

$n\ total = 1 + 1 = 2$

(لما بفرق عن x لأنه ما عندي قيمة y وعندي قيمة x)

2.

A → 100 Ibm/min B → 300 Ibm/min

$M_A = 2$ $M_B = 3$

$x_A = \frac{m_A}{m\ total} = \frac{100}{400} = 0.25$ Ibm A / Ibm

$x_B = \frac{m_B}{m\ total} = \frac{300}{400} = 0.75$ Ibm B / Ibm

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$$y_A = \frac{n_A}{n_{total}}$$

$$= \frac{50}{150} = 0.333 \text{ mole A/mole}$$

$$n_A = \frac{m_A}{M.w} = \frac{100}{2} = 50$$

$$n_B = \frac{300}{3} = 100$$

$$n_{total} = 150$$

$$y_B = \frac{n_B}{n_{total}} = \frac{100}{150} = 0.666 \text{ mole B/mole}$$

mass flow rate of A? given ⟶ 100 Ibm/min

molar flow rate of B?

n_B /min = 100 Ib mole /min

Total mass flow rate?

$m_A + m_B$ = 400 Ibm 400 Ibm /min

Total molar flow rate?

$n_A + n_B$ = 150 ⟶ 150 Ib mole /min

Concentration:

Mass Concentration: Mass of component per unit volume.

[g/cm³, Ibm/ft³, Kg/in³]

Molar Concentration: Number of moles of the Component per unit volume. [Kmol/m³, Ib-moles/ft³, gmol/cm³]

Molarity: The value of molar concentration of the solute expressed in g moles Solute/Liter Solution.

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Concentration can be used as conversion factor to relate mass or moles to the volume, or to relate mass or molar flow rate to total volumetric flow rate.

Test yourself p: 52

1. $n/V \rightarrow$ moles/L
2. $n \cdot M/V \rightarrow$ g/L
3. $20 \text{ moles} \times \frac{L}{CA \text{ moles}} = 20/CA \text{ L}$
4. mass flow = ? (g/h)

   volumetric flow = 120 L/h

   $120 \frac{L}{h} \times \frac{CA \text{ g}}{L} = 120 CA \text{ g/h}$

Parts per Million and parts per Billion.

$ppm\ i = y_i \times 10^6$ $\quad$ $ppb\ i = y_i \times 10^9$

Test yourself p:54

1. $x = \frac{m \text{ phenol}}{m \text{ Liquide}} = \frac{125 \text{ g}}{10^9 \text{ g}} = 125 \times 10^{-9}$

2. $\frac{125 \text{ g phenol}}{10^9 \text{ g Liquide}} \times \frac{1000 \text{ g}}{1} \times \frac{1000 \text{ mg}}{1 \text{ g}} = 125 \times 10^{-3} \text{ mg}$

3. Concentration in g/L ? $\quad \rho_{water} = 1.07 \text{ g/cm}^3$

   $\frac{125 \text{ g phenol}}{10^9 \text{ g Liquid}} \times \frac{1.07 \text{ g Liquid}}{\text{cm}^3} = 1.34 \times 10^{-7} \text{ g/cm}^3$

   $\frac{1.34 \times 10^{-7} \text{ g}}{\text{cm}^3} \times \frac{10^6 \text{ cm}^3}{1 \text{ L}}$

   $= 134 \times 10^{-6} \text{ g/L}$

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Temperature

Relative temperature scale: " نسبية "

- Celsius : 0°C (Freezing point for water) ⟶ 100°C B.P
- Fahrenheit: 32 ⟶ 212 B.P
  Freezing point

From °C to °F :

$$T_f = 1.8 \times T_c + 32$$

From °F to °C :

$$T_c = \frac{T_f - 32}{1.8}$$

Absolute temperature scale:

- Kelvin
- Rankine

• Reading of zero coincides with the theoretical absolute zero (entropy = zero)

From °C to K

$$T_K = T_c + 273.15$$

From F to °R

$$T_R = T_f + 459.67$$

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Pressure

$$\text{pressure} = \frac{\text{force}}{\text{area}}$$

N / m^2 (SI) It's called pascal (Pa)

$dynes / cm^2$ (CGS)

lbf / in^2 (American engineering) psi

Atmospheric pressure: (Barometric pressure)

The pressure of the surrounding air, local pressure of the atmosphere.

- pressure at the base of a column of air.
- Atmospheric pressure decreases with increasing in elevation (ارتفاع).

Absolute pressure (Pabs):

- pressure measured relative to a fixed reference point of zero pressure. (vaccume : no molecules).

Gauge pressure (P_g):

pressure relative to the atmospheric pressure.

زيادة أو نقصان عن ال atm pressure.

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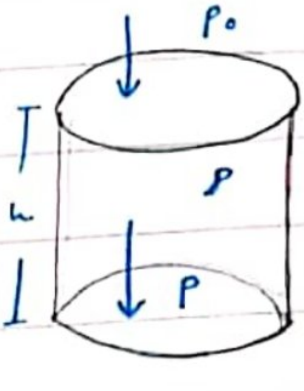
Hydrostatic pressure : The pressure of a fluid at the base of the column, (not moving column of water)
= force on top + weight of the fluid in the column.

$$P = P_0 + \rho g h$$

- P ← pressure at the bottom of the liquid
- P_0 ← top of column
- ρ ← density of fluid
- g ← acceleration (gravity)
- h ← height



ρ water = 1.07 g/cm³

اذا كان ال fluid داخل column هو الماء اذا يكون hydrostatic pressure ، اذا كان نوع آخر من fluid بطبق على نفس القانون ولكن بال density الخاصة بهذا ال fluid .

Head pressure :

$$\frac{P}{\rho g} = \frac{P_0}{\rho g} + \frac{\rho g h}{\rho g}$$

(اذا كان نفس ال نوع)

$$ph = pho + h$$

(لها units علاقة بالأطوال)

Test your self p: 56

1. تعاريف عادية ←

2. $P = P_0 + \rho g h$, pressure is higher at the bottom than the top. $P - P_0 = \rho g h$

ρ air = 1 kg/m³ ρ water = 10^3 kg / m³ ρ mercury = 13600 kg/m³

If fluid was air → No, because it's density is

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$P_{absolute} = P_{gauge} + P_{atmospheric}$

psig = lbf/in^2 gauge pressure.

psia = lbf/in^2 absolute pressure.

— Using of absolute pressure:

- In a formula like ideal gas equation $PV = nRT$
- Taking ratios of pressure.

— Use gauge pressure when:

- Taking differences in pressure $\Delta P_{guage} = \Delta P_{absolute}$

Note: p_{atm} = 1 atm = 760 mm Hg = 101.3 kpa = 29.92 in Hg
= 33.91 ft H_2O = 14.7 psi (lbf/in^2)

If patmospheric is not given we use the standard atmospheric pressure.

$$\text{Head pressure} = \frac{P}{\rho g}$$

↓
بدلالة الـ fluid المراد التعبير عنه

طول :

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very small.

$(P - P_o)$ mercury $> (P - P_o)$ water $> (P - P_o)$ air

h → ρ

فإذا كان الارتفاع قليل سيكون P قليل ايضاً. | لأنه كثافته عالية جداً، بغض النظر عن الارتفاع.

3. $A = 4\ cm^2$ $\qquad F = ?$ $\qquad F = P \times A$

$P = 1300\ mmHg$

$$\times \frac{1.01325 \times 10^5\ N/m^2}{760\ mmHg} \times 4\ cm^2 \times \left(\frac{1\ m}{100\ cm}\right)^2$$

=

4. $74\ mmHg$ $\quad P_o$] $h = 5\ mm$, $P = ?$

$P = P_o + \rho g h$

$$= 74\ mmHg \times \frac{1.01325 \times 10^5\ N/m^2}{760\ mmHg} + 13600\ \frac{kg}{m^3} \times 9.8\ \frac{m}{s^2} \times 5\ mm \times \frac{0.001\ m}{1\ mm}$$

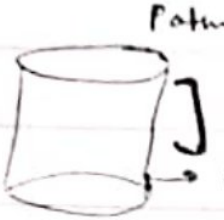
$$= 10.5 \times 10^3\ N/m^2 \simeq 79\ mmHg$$

3. $P_{absolute} = -20 + 755 = 753$ mmHg

P = 20 mm Hg of vaccume

Patmospheric يو يزل 20 mm

4.



$P_g > P_{atm}$

$P_g = +4$ in Hg

$P_{absolute} = 4 + 29.9 = 33.9$ in Hg

Pressure measurments:

- **Bourdon gauge:**
  - Hollow tube closed at one end.
  - The open end of the tube is exposed to the fluid whose pressure is to be measured
  - As the pressure increase, the pointer attached to the tube will rotate, and the tube tends to straighten.
  - measure the gauge pressure.
  - measure fluid pressures from perfect vaccums to 7000 atm.

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- Atmospheric pressure can be calculated as the pressure at the base of column, by assuming that the pressure at the top (P_0) = zero

$$P = P_0 + \rho g h$$

$$\rightarrow P_{atm} = \rho g h$$

- when gauge pressure = 0, it means that the absolute pressure is equal to atmospheric pressure.

For converting between absolute and gauge pressure:

$$P_{absolute} = P_{gauge} + P_{atmospheric}$$

- when refering to negative gauge pressure, as positive amounts of vaccum → -1 cm Hg = P_{gauge} (P_{atm} = 76 cm Hg, $P_{absolute}$ = 75 cm Hg) and 1 cm of vaccume.

Test yourself 56, 57

1. NO

2. absolute : pressure of zero corresponds to vaccume.
   gauge : pressure relative to atmospheric pressure.

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Manometers

- measurments of pressure below 3 atm.
- U shaped tube partially filled with a fluid of known density.
- Both ends of the tube are exposed to different pressures causing differences in the level of the manometer fluid in both arms.
- Difference between pressure can be calculated from the difference between the liquid levels of each arm (h_2)

open-end: one is exposed to a fluid whose pressure is to be measured, and the other is opened to the atmosphere, difference in height will be the gauge pressure because it's related to P_{atm}.

Differential: measures the pressure difference between two points in a process line.

Sealed - end: enclosed at one end $P_2 = 0$
(measure the difference between P and zero
→ Absolute pressure

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General manometer equation:

$$P_1 + \rho_1 g d_1 = P_2 + \rho_2 g d_2 + \rho_f g h$$

(point 1 = point 2)

Differential manometer : fluids 1 and 2 are the same so $\rho_1 = \rho_2 = \rho$

$$P_1 - P_2 = (\rho_f - \rho) g h$$

* ρ_f : manometer fluid density.

If both fluids are gases:

$$P_1 - P_2 = \rho_f g h \qquad \rho \ll \rho_f$$

$h = P_1 - P_2$ ✓

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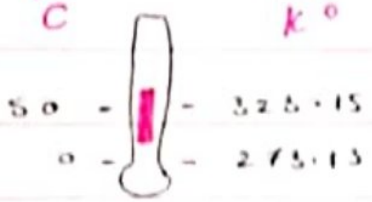
°C K°



$T_K = T_C + 273.15$ $T_F = 1.8\,T_C + 32$

$1c^\circ\,(diff) = 1K\,(diff)$ $1c^\circ\,(diff) = 1.8F\,(diff)$

From F to R°

$T_{R^\circ} = T_F + 459.67$

K° to R

$T_R = 1.8\,T_K$

Unit temperature difference:

$\Delta C^\circ = \Delta K$ $\Delta F^\circ = \Delta^\circ R$

but $\Delta C^\circ = 1.8\,\Delta f$ $\Delta K = 1.8\,\Delta R$

$$\Delta T = \frac{1.8F^\circ}{1c^\circ}, \frac{1.8R^\circ}{1K}, \frac{1F^\circ}{1R^\circ}, \frac{1c^\circ}{1K}$$

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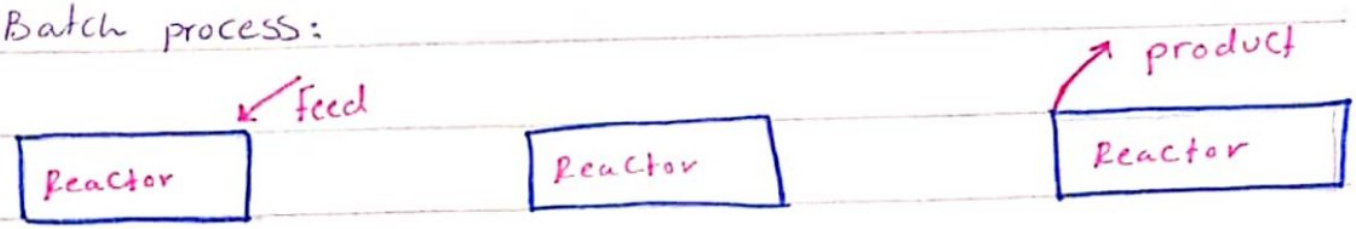
CH: 4 Fundamentals of Material Balances

Process: A series of operations involving the physical, chemical and biological transformation of an input material for the purpose of achieving a desired product material.

- we have 3 types of chemical processes:

1. Batch process 2. Continuous process 3. Semi batch process.

Batch process:



All materials are added at the start of the process, then the process is allowed to proceed, products are withdrawn after completion of the process, No mass crosses system boundaries (closed system), batch processing is used when small quantities are to be produced.

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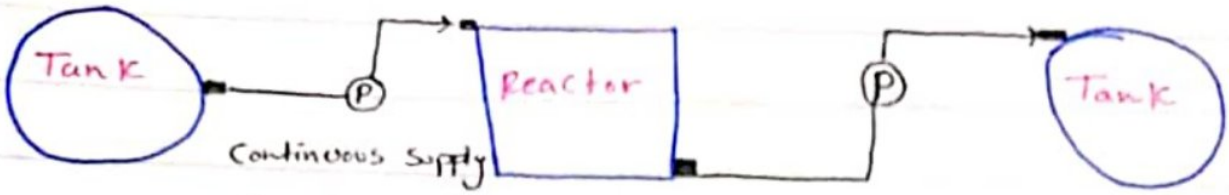
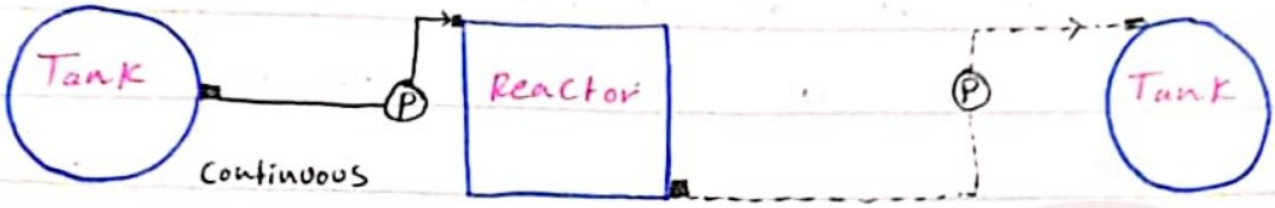
Continuous process :



of feed (input) Continuous with drawal of product.

- Inputs and outputs flow continuously through the process, mass crosses system boundaries (open system) (خلال العملية في سواد داخلة وخارجة).
- Continuous process is used with large production rates

Semi batch process (semi continuous).



supply of feed product with drawn at the end of the process

- process that's neither batch nor continuous
- process اما عندي continuous supply of feed ويتم سحب النواتج نهاية الـ feed is charged and the product is continuously withdrawning. او (واحد منهم يكون بشكل مستمر).

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Steady state :

- No change within time to all variables in a process (temperatures, pressures, volumes, flow rates).
- Continuous process may be steady state.

Unsteady State (transient)

- If any of the process variables change with time.
- Batch and semi batch processes are unsteady by their nature.
- Continuous may be transient also (unsteady).

Test yourself p: 84

- Semi batch – transient ← في تغير بمرور الزمن ← (بدخل الهوا)
- Batch – transient (تغير في درجة الحرارة)
- Semi – batch – transient (No input but there's output (بخار الماء))

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General balance equation

on any conserved quantity:

Input + generation − out − consumption = accumulation

Input: enters through system boundaries

generation: produced within system.

output: leaves through system boundaries

consumption: Consumed within system

Accumulation: build up within system (تراكم)

Types of balances:

1. Differential balances: describes what's happening in a system at an instant of time.

- each term of the balance is a rate.
- Has units of balanced quantity per time (people/yr , gSO_2/s)
- usually applied to a continuous process.

Integral balances: describes what happens between 2 instants of time.

- each term of the balance is an amount of the balanced quantity (no rate) " people , gSO_2 "

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- usually applied to batch process.

To simplify the material balance equation:

- If balance quantity is total mass : (conserved quantity)

set generation = 0 and consumption = 0

Input − output = accumulation

- If balanced substance is non reactive species (inert)

generation = 0 consumption = 0

Input − output = accumulation.

- If a system is steady state

no accumulation or depletion : within system

set accumulation = 0

- total mass or non reactive at steady state

Input = output.

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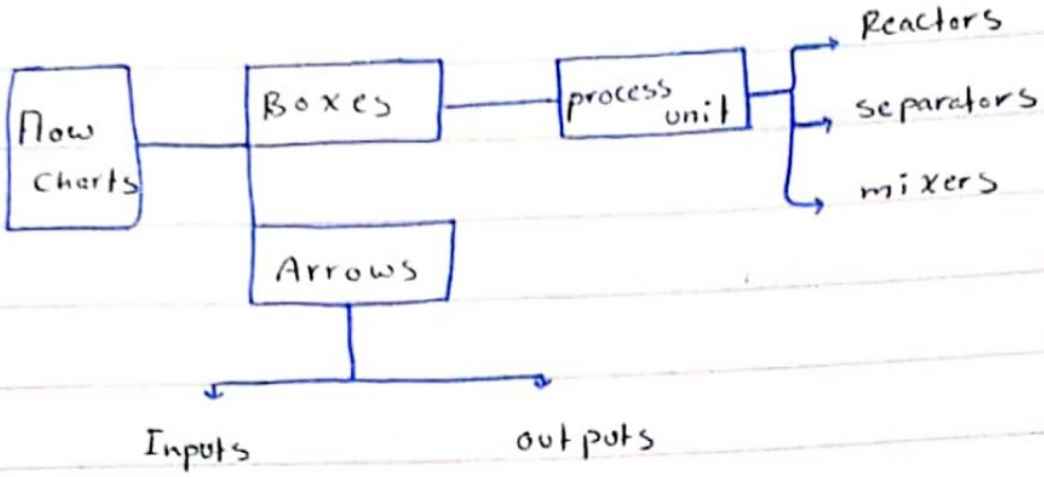
Material balance calculations

Flow charts:

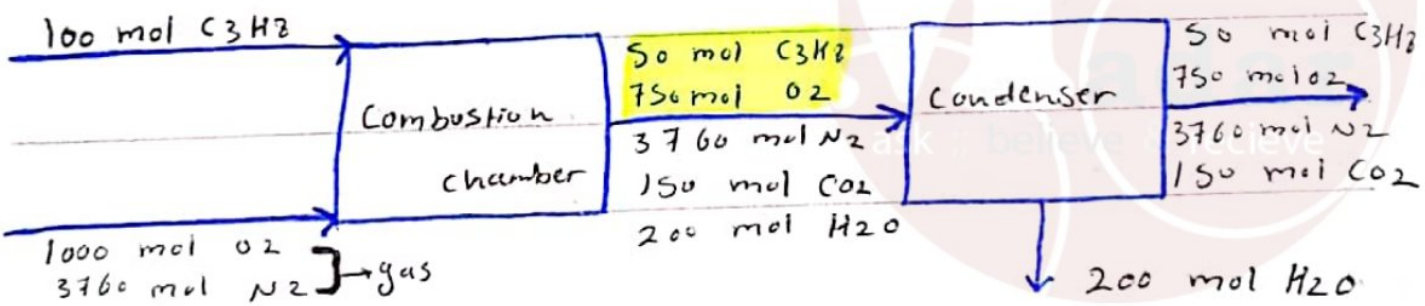
. To organize the information in a way that is convenient for subsequent calculations.



Labelling the Flow chart:

- values for known process variables.
- symbols for unknown variables.

. A gas containing N_2 and O_2 is combined with propane (C_3H_8) in a batch combustion chamber, some (but not all) of the O_2 and C_3H_8 react to form CO_2 and H_2O, the product is then cooled, condensing the water.



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To have a helpfull lablled flow chart:

- write the values and units of all known stream variables at the locations of the streames on the chart. (اكتب كل المعطى مع وحداتهم)

400 mol / h
→
0.2 mol O_2/mol
0.79 mol N_2/mol

T = 32 °C , p = 1.4 atm

- we have 2 ways:

→
60 kmol N_2/min
40 kmol O_2/min

=

100 k mol/min
→
0.6 kmol N_2/kmol
0.4 kmol O_2/kmol

. يا total "فوق السهم" وال composition (mol or mass fractions) تحت
او كميات كل مادة "تحت السهم".

- Assign symbols to unknown streams variables with their units.

$\dot{n}$ (mol/h)
→
0.21 mol O_2/mol
0.79 mol N_2/mol
T = --- , p = ---

. known composition
. unknown total amount

400 mol / h
→
y mol O_2/mol
1−y mol N_2/mol

. know total amount
. unknown composition

Test yourself p: 93

2. $\dot{m}_{total} = 250\ kg/h$, $\dot{m}$ (kg/min) for C_7H_8 ?

$$x = \frac{\dot{m}\ C_7H_8}{\dot{m}\ total} \quad / \quad 250(1-x)\ \frac{kg}{h} \times \frac{1\ h}{60\ min} = \frac{250(1-x)}{60}$$

3. $V = 75\ ml$ $n = ?$

$\rho = 1.595\ g/cm^3$

$M.w = 154\ g/mol$

$$1\ ml = 1\ cm^3$$

$$75\ ml \times \frac{1\ cm^3}{1\ ml} \times \frac{1.595\ g}{cm^3} \times \frac{1\ mol}{154\ g}$$

$$n = 0.766\ mols.$$

4. $\dot{m}$ (kg total/s)

$\dot{m}\ CO$ (kg CO/s)

g = kg CO_2 / kg total)

$$\dot{m}\ total = \dot{m}\ H_2O + \dot{m}\ dg$$

$$\dot{m}\ total = 50\ kg\ H_2O/s + \dot{m}\ dg \ \ kg\ dry\ gas/s$$

$$x \frac{\dot{m}\ dg\ kg\ dry}{s} = 0.25\ kg\ CO/s$$

$$\frac{kg\ CO_2}{kg\ total} = \frac{0.75}{50 + \dot{m}\ dg}$$

Rules applied to non-reactive processes:

1. number of independent equations that can be derived by writing balances on a nonreactive system = number of chemical species in the output and input streams.

2. write balance first that involve the fewest unknown variables.

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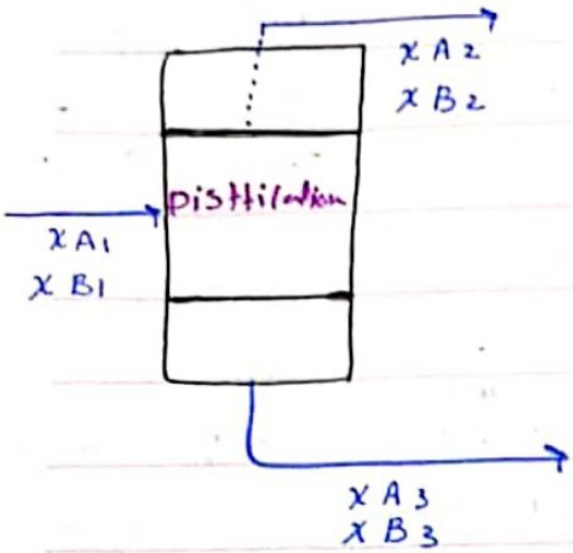
Non reactive → generation and consumption = 0 .

Steady state → accomulation = 0 .

Steady - state distillation process:



① • يتم فصل اذ stream ، وكل component

تكون كمية أكبر من الأخرى مثلاً :

In stream 2 : $x_B < x_A$

In stream 3 : $x_B > x_A$

Cases:

- Component mass or mole fractions → variable's names need to be assigned to all but one fraction

x_1

x_2

$x_3 \rightarrow 1 - (x_1 + x_2)$

- 3 times N_2 (by mass) in a Stream as O_2 → $y_{O_2} = 3y$ (not y_1 and y_2)

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- volumetric flow rate of a stream is given ⟶ convert it to mass or molar flow rate

(we don't use volume balance : only mass or mole balance)

- Basis of calculation is an amount or flow (mass/molar) of one stream or component in a process.

- If no stream amounts or flows are known, assume value of only one stream: How?

1- If mass fractions are known ⟶ set total mass or $\dot{m}$

2- If mole fractions are known ⟶ set total number of moles or $\dot{n}$.

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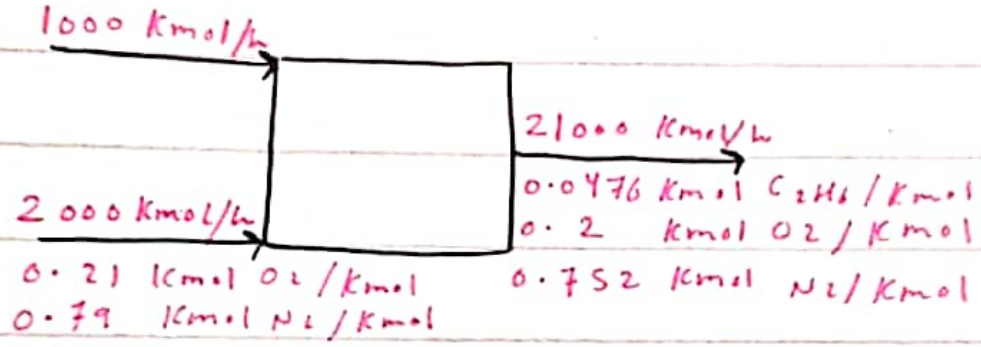
Test yourself p: 95

2.

a. Scale factor = $\frac{1000 \text{ Kmol/h}}{100 \text{ mol}} = \frac{10 \text{ Kmol/h}}{\text{mol}}$

- 100 mol × $\frac{10 \text{ Kmol/h}}{\text{mol}}$ = 1000 Kmol/h
- 20000 Kmol/h and the product = 21000 Kmol/h
- mol fractions stays the same. (convert their units)



b.

Scale factor = $\frac{100 \text{ Ibm/min}}{1 \text{ g}} = 100 \frac{\text{Ibm}}{\text{g.min}}$

- 1g ⟶ 100 Ibm/min
- 0.5 g ⟶ 50 Ibm/min
- , , , ⟶ 50 Ibm/min
- mass fractions doesn't change. (only convert the units)

Test yourself p: 98

1.

H_2 balance

$10 \times 0.5 = 0.2 \times S + Y$

S Ibm H_2 / Ibm $=$ S Ibm H_2 / Ibm

O_2 balance

$0.5 \times 10 = 0.8 \times S + 1$

$S = S$

total balance

$10 = S + m$

$m = 5$ Ibm

2.

Total balance :

$m'_1 + m'_2 = 400$ g/s ----- (1)

B balance :

$0.2\, m_1 = 400 \times 0.1$ ----- (2)

$m_1 = 400 \times 0.1 / 0.2 = 200$ g/s

C balance :

$0.5 \times 200 = 400\,(0.9 - x)$ ----- (3)

$100 = 360 - 400\, x$

$x = 0.65$ g A / g

Degree of freedom analysis (DoF)

1. Draw and completely labelled a flow chart.
2. Count the unknown variables on the chart (n unknown)
3. Count the independent equations relating them (n indep eqns)
4. Calculate the degree of freedom of the process

DoF = nonknown - n indep eqns

- Sources of equations in DoF analysis.

- Independent material balance equations = number of species
- Stoichiometric relations based on chemical reactions
- physical constraints on some variables ($x_B = 1 - (x_A + x_C)$)
- process specifications.
- physical properties and laws.
- Energy balance equations.

If:

DoF = 0 problem can be solved

DoF > 0 at least 'DOF' additional variables must be specified. Ex; DoF = 3 (يحتاج 3 معلومات اضافية)

DoF < 0 Flow chart is incomplete, the problem is

Over-Specified (حتى معلومات مكررة)

Hints on DoF:

- use flow rates instead of fractions.
- one species mass or mole fraction is not independent ($\sum x_i = 1$, $\sum y_i = 1$) مثلاً $x_A = 1 - x_B$
- If only one fraction is unknown in a stream, calculate it and treat it as known.
- It's easiest to use the total mass balance as 1 equation instead of all the species balances.

حتى 3 species مثلاً A, B, C :

اكتب معادلة total balance, معادلتين لـ species بدل species من 3 معادلات.

- use the flow rate given as the basis.

اذا ماحتى أي flow rate يختار (فرض) ← basis ممكن 100 kg/h, 100 mol/h حسب الـ components الموجودة

- افرض حسب الـ stream الذي فيه أكبر قدر من المعلومات عن الـ components.

- If you know the densities and volumetric flow rates calculate the mass flow rates immediately.

General procedure for single-unit process Material balance.

1. Choose a basis of calculation
   (an amount or flow rate of one of the streams).
2. Draw and label the flow chart.
   - Fill in all known values, including the basis of calculation
   - Label unknown stream variables on the chart.
3. write expressions for the quantities requested in the problem.
   (كتابة المطلوب ايجاده من السؤال)
4. Convert mixed units (mass and mole units)
   (توحيد الوحدات اما بـ mass أو mole)
5. Calculate degree-of Freedom.
6. If DOF=0, write the equations in an efficient order
   التقليل من حل المعادلات مع بعض البعض، والحصول على مجهول واحد
   في كل معادلة.
7. Solve the equations.
8. Calculate the quantities requested in the problem

4-4 Balances on multiple - unit processes:

- **System**: is any portion of a process that can be enclosed within a hypothetical box (boundary) it may be entire process, combination of some units (units مجموعة) or a point at which 2 or more process streams come together, (mixing point) or one stream splits into branches (splitting point).

- The inputs and outputs to a system are the process streams that intersects the system boundary.

- when analyzing multiple - unit processes, find the DoF on the overall process and on each subsystem.

- Start solving when DoF = 0.

4.5

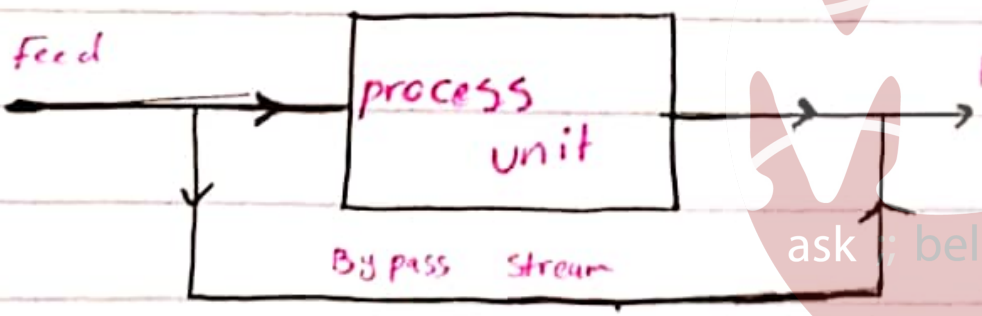
Recycle and Bypass.

Reasons for using recycle :

1. recouring (reusing) unconsumed reactants.
2. recovery of catalyst. (it may be recovered with the unconsumed reactants or separately in special facilities).
3. Dilution of a process stream, (If the concentration of solids is too high → we recycle the filtrate to dilute the feed).
4. control of process variable, (heat of generation can be reduced by lowering the concentration of the reactants).
5. circulation of a working fluid.

Bypass:

a fraction of the feed to a process unit is diverted around the unit and combined with the output stream.



4.6 Chemical reaction stoichiometry

Stoichiometry is the theory of the proportions in which chemical species combine with one another.

Stoichiometric equation: a statement of a relative number of molecules or moles of reactants and products that participate in the reaction.

$$\boxed{2}\ SO_2 + O_2 \longrightarrow 2SO_3$$

↓ Stoichiometric Coefficient

2 mols of SO_2 : 1 mol of O_2 : 2 mols of SO_3

(g-mol, lb moles)

Stoichiometric ratio: is the ratio of their stoichiometric coefficients in the balanced equation.

It can be used as a conversion factor to calculate the amount of particular reactant or product that was consumed or produced.

Test yourself p: 117

1. C: $4 \times 1 = 4$ ✓

H: $4 \times 2 = 8$ ✓

O: $4 \times 2 + 4 \times 1 = 12$ ✓

It's balanced

2. 4

3. $\frac{4\ H_2O}{6\ O_2}$ · $\frac{2\ H_2O}{3\ O_2}$

· 400 lb-moles CO_2 × $\frac{6\ \text{lb-moles}\ O_2}{4\ \text{lb-moles}\ CO_2}$ = 600 lb-mole O_2

5. So C_4H_8 $\frac{\text{mol reacted}}{\text{min}}$ × $\frac{4\ H_2O\ \text{mol produced}}{1\ C_4H_8\ \text{mol reacted}}$ = 200 mol/min

4.6 b Limiting and excess reactants

$$A + 2B \longrightarrow C$$

$\frac{\text{moles A}}{\text{moles B}}$ = 1/2 = stoichiometric ratio

Fractional excess of A: $\frac{(nA)\ \text{Feed} - (nA)\ \text{St}}{(nA)\ \text{Stoich}}$

percent excess of A = 100% x fractional excess

fractional conversion = f = $\frac{\text{moles reacted}}{\text{moles fed}}$

percentage Conversion = $f \times 100\%$

Note: reaction don't usually proceed to completion.

Extent of reaction $\xi = ni - nio / vi$

ni = exit moles of i

nio = feed moles of i

vi = stiochiometric. coff. of i

(product) + − (reactant)

. each reaction has one value of (extent of reaction), It's always (+), ξ has the same unit of n.

Test your self p: 119

1. Feed ratio = 1 C_2H_4 / 1 O_2 Stoichiometric ration = 2 C_2H_4 / 1 O_2

(C_2H_4 is the limiting reactant)

2. % excess of O_2 = 100 − 50/50 = 100 %

3. $100\ Kmol\ C_2H_4 \times \frac{1\ Kmol\ O_2}{2\ Kmol\ C_2H_4} = 50\ Kmol\ O_2$

$100\ Kmol\ consumed \times \frac{2\ mol\ formed}{2\ Kmol\ consumed} = 100\ Kmol\ C_2H_4O$

$\xi = 0 - 100 / -2 = 50\ Kmol$

4. f = reacted / feed

$$0.5 = \frac{n_{A_0} - n_A}{n_{A_0}}$$

$0.5 = 100 - n_A / 100$ ⇒ $n_A = 50$ kmol

$\xi = 50 - 100 / -2 = 25$ kmol

$\xi = \frac{n_B - n_{B_0}}{\nu_B}$ ⇒ $25 = n_B - 100 / -1$ $n_B = 75$ kmol

$\xi = n_C - n_{C_0} / \nu_C$ $25 = n_C - 0 / 2$ $n_C = 50$ kmol

5.

$f_{O_2} = 100 - 60 / 100 = 0.4$

$\xi = n_B - n_{B_0} / \nu_B = 60 - 100 / -1 = 40$ kmol

$\xi = n_A - n_{A_0} / \nu_A$ ⇒ $40 = n_A - 100 / -2$ $n_A = 20$ kmol

$f_A = 100 - 20 / 100 = 0.8$

4.6c Chemical equilibrium

1- what will be the final (equilibrium) composition of the reaction mixture ? Chemical equilibrium thermo dynamics.

2- How Long will the system take to reach a

Specified state short of equilibrium?

(Chemical kinetics)

Reactions

reversible

- $R \rightleftharpoons P$

irreversible

- reaction proceeds in a single direction from (R to P)
- concentration of limiting reactant $\simeq 0$

4-6 d Multiple reactions, yield and selectivity

$$C_2H_6 \longrightarrow C_2H_4 + H_2$$

side reactions:

$$C_2H_6 + H_2 \longrightarrow 2\,CH_4$$

$$C_2H_4 + C_2H_6 \longrightarrow C_3H_8 + CH_4$$

Yield, **Selectivity** are used to describe the degree to which a desired reaction predominates over competing side reactions.

Yield = moles of desired product / moles that would've been formed with no side reactions and L.R had completly reacted.

Selectivity: $\frac{\text{moles of desired product}}{\text{moles of undesired product}}$

Extent of reaction

$$n_i = n_{io} + \sum_j \nu_{ij} \xi_j$$

Test your self p: 125

1. $f_A = 100 - 10 / 10 = 0.9$

2. yield of B % = $160 / 200 \times 100\% = 80\%$

3. $160 / 10 = 16$ mol B / mol C

4. $n_A = n_{A_0} + (\xi_1 (-1)) + \xi_2 (-1)$

$10 = 100 - \xi_1 - \xi_2$

$10 = 100 - 80 \xi_2$ $\quad 10 = 20 - \xi_2$

$\xi_2 = 10$ mol

$$n_B = n_{B0} + (\xi_1 (2) + \xi (0))$$

$$100 = 2\xi_1 + 0$$

$$\xi_1 = 80 \text{ mol}$$

$$n_C = n_{C0} + 0\,\xi_1 + \xi_2 (1)$$

$$10 = \xi_2 \longrightarrow \xi_2 = 10 \text{ mol}$$

Test yourself p:128

1. 3 independent molecular species (C_2H_4, N_2, C_4H_8)

   2 atomic independent species (C or H , N)

- C balance: $2 \times 0.6 \times 100 = 2n_1 + 4n_2$ } نفس المعادلة
- H balance: $4 \times 0.6 \times 100 = 4n_1 + 8n_2$
- N balance: $2 \times 0.4 \times 100 = 2n_3$

ratio بين H و C ← 2 سواء ب C_2H_4 او C_4H_8. عشان هيك نفس ال ratio
ف هم مش independent.

2. $CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$

   $CH_4 + \frac{3}{2}O_2 \longrightarrow CO + 2H_2O$

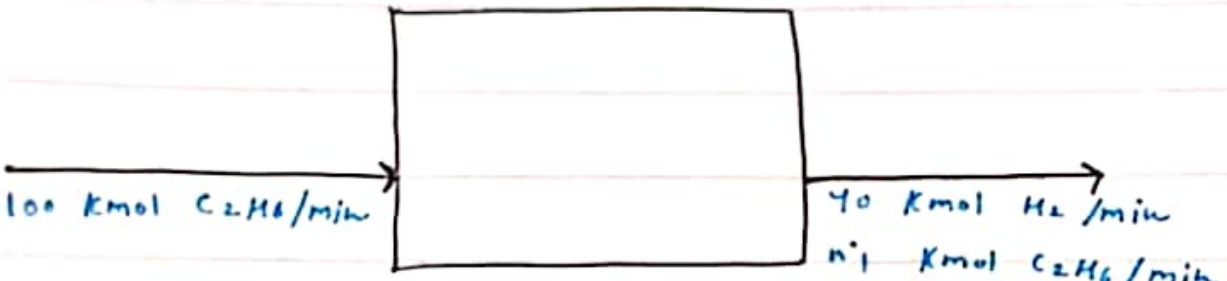
   $C_2H_6 + \frac{7}{2}O_2 \longrightarrow 2CO_2 + 3H_2O$

   $C_2H_6 + \frac{5}{2}O_2 \longrightarrow 2CO + 3H_2O$

Solving methods for a reactive system

Molecular Balance	Atomic balance	Extent of reactions.
- includes the terms: composition / generation . used only for simple systems (1 or 2 reactions).	• when more than 1 reaction is involved • doesn't depend on the reaction itself. (Input = output) "at steady state"	($n_i = n_{i0} + \sum \nu \xi$)

(Input + generation = output + consumption)



$[C_2H_6 \longrightarrow C_2H_4 + H_2]$

Molecular species balance:

DoF =

+ 2 unknowns

+ 1 Chemical reaction

− 3 molecular species

DoF = 3 − 3 = 0 ✓

H_2 balance:

generation of H_2 = 40 Kmol /min

C_2H_6 balance:

Input + generation = output + consumption

$100 = n'_1 + 40$ $\quad n'_1 = 60$ Kmol /min

C_2H_4 balance:

0 + 40 = n'_2 $\quad n'_2 = 40$ Kmol/min

generation ✓

Atomic Species balance:

+ 2 unknowns

− 2 atomic species balance (C, H)

DoF = 2 − 2 = 0

(ما الي reaction بال بالسؤال)

Carbon balance : $100 \times 2 = 2\dot{n}_1 + 2\dot{n}_2$ $\quad 100 = \dot{n}_1 + \dot{n}_2$

$\dot{n}_1 = 100 - \dot{n}_2$ ... (1)

Hydrogen balance: $6 \times 100 = 6\dot{n}_1 + 4\dot{n}_2 + 2 \times 40$

$600 = 6(100 - \dot{n}_2) + 4\dot{n}_2 + 80$

$600 = 600 - 6\dot{n}_2 + 4\dot{n}_2 + 80$

$-80 = -2\dot{n}_2$ $\quad \dot{n}_2 = 40$ kmol /min

$\dot{n}_1 = 100 - 40 = 60$ kmol /min

Extent of reaction:

$n_i = n_{i0} + \Sigma \nu \xi$

+ 2 unknowns

+ 1 chemical reaction

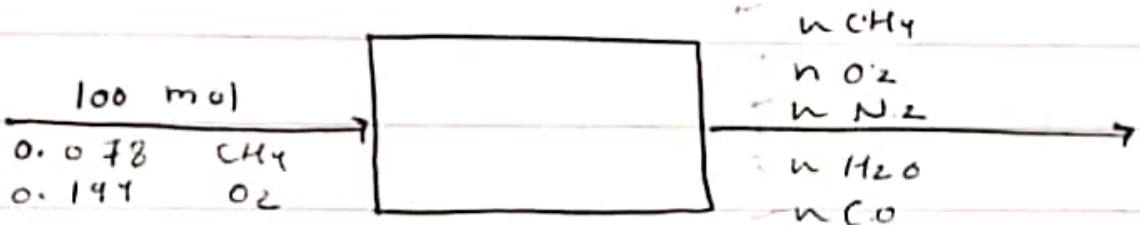
− 3 molecular species

DoF = 3 − 3 = 0 ✓

H_2 balance: $40 = 0 + \xi$ $\quad \xi = 40$ kmol /min

C_2H_6 balance: $n_i = 100 - 40 = 60$ kmol /min

Example 4.7-1



- $\frac{n\ CO_2}{n\ CO} = 8$ — 90% conversion

$n_{CO_2} = 8CO$

- Molecular Species balance:

unknowns: 5 Reactions: 2

molecular species: 6 relations: 1 (90%)

DoF = 7 - 7 = 0

- Extent of reaction:

unknowns = 5 Reactions = 2

reactive = 5 non reactive = 1

relations = 1

DoF = 7 - 1 = 0 ←

(reactions عدد)

- Atomic Species balance:

unknowns = 5 Atoms = 3 (C, H, O)

non reactive molecules = 1 (N_2) relations = 1

DoF = 5 - 5 = 0

Conversion = $\frac{In - out}{In}$

for CH_4

$0.9 = \frac{7.8 - n_{CH_4}}{7.8}$

$n_{CH_4} = 0.78$

Nitrogen balance

$n_{N_2} = 0.728$ mol N_2/mol

(because Hrs are inert)

Molecular species balance:

. I need consumption and generation for each reaction. [Input + generation = output + consumption]

CH_4 balance:

$0.078 \times 100 = CH_{4(1)} + CH_{4(2)} + 0.78$ ---(1)

CO_2 balance:

$0 + CO_2$ generation $= n_4 + 0$

CO balance:

$0 + CO$ generation $= n_{CO} + 0$

CH_4 (1) consumption = CO generation

CH_4 (2) consumption = CO_2 generation } ratio 1:1

So $n_{CO} = CH_4$ (1)

$n_{CO_2} = CH_4$ (2)

$7.8 = n_{CO} + n_{CO_2} + 0.78$

$7.8 = n_{CO} + 8\,n_{CO} + 0.78 \rightarrow n_{CO} = 0.78$

$n_{CO_2} = 8 \times 0.78 = 6.24 \text{ mol}$

O_2 balance:

n_{CO}

$0.194 \times 100 + 0 = n_{O_2} + \frac{3}{2}$ Consumption CH_4 ① + 2 Consumption CH_4 ②, n_{CO_2}

$19.4 = n_{O_2} + \frac{3}{2} n_{CO} + 2 n_{CO_2}$

$19.4 = n_{O_2} + 3/2 \times 0.78 + 2 \times 6.24$

$\rightarrow n_{O_2} = 5.75 \text{ mol}$

H_2O balance:

$0 + 2$ CH_4 ① consumption + 2 CH_4 ② consumption = $n_{H_2O} + 0$

$2 \times 0.78 + 2 \times 6.24 = n_{H_2O}$

$n_{H_2O} = 14.04 \text{ mol}$

$n_{total} = n_{dry} + n_{H_2O}$ ---- $= 100.4 \text{ mol}$

$y_{O_2} = -$ $y_{CO_2} = -$ $y_{CO} = -$

Extent of reaction method

2 reactions $\longrightarrow$ 2 ξ

ξ_1 and ξ_2 = ?

$[n_i = n_{i0} + \Sigma \nu \xi]$

CH_4 : $0.78 = 7.8 - \xi_1 - \xi_2$

CO : $n_{CO} = 0 + \xi_1$

CO_2 : $n_{CO_2} = 0 + \xi_2$

$n_{CO_2} = 8\, n_{CO}$

$0.78 = 7.8 - n_{CO} - n_{CO_2}$

$0.78 = 7.8 - n_{CO} - 8\,n_{CO}$

$n_{CO_2} = 8 \times 0.78 = 6.24$

$-7.02 = -9\, n_{CO}$

$n_{CO} = 0.78$ mol

$\xi_1 = 0.78$ $\xi_2 = 6.24$

O_2 : $n_{O_2} = 19.4 - 3/2\, \xi_1 - 2\xi_2$

$n_{O_2} = 19.4 - 3/2\,(0.78) - 2(6.24)$

$n_{O_2} = 5.75$ mol

H_2O : $n_{H_2O} = 0 + 2\xi_1 + 2\xi_2$

$n_{H_2O} = 14.04$

Atomic Species balance

(یعنی بدون نیاز از reaction)

Carbon balance :

$n_{CO_2} = 8 n_{CO}$

$0.078 \times 100 = \underbrace{0.78}_{n_{CH_4}} + n_{CO_2} + n_{CO}$

$7.8 = 0.78 + 8n_{CO} + n_{CO}$ $\quad 7.8 = 0.78 + 9n_{CO}$

$n_{CO} = 0.78$ mol

$n_{CO_2} = 8 \times 0.78 = 6.24$ mol

H balance :

$4 \times 0.078 \times 100 = n_{CH_4} \times 4 + n_{H_2O} \times 2$

$31.2 = 3.12 + 2n_{H_2O}$

$n_{H_2O} = 14.04$ mol

Oxygen balance :

$0.194 \times 2 \times 100 = 2 \times n_{O_2} + n_{CO_2} \times 2 + n_{CO} + n_{H_2O}$

$38.8 = 2n_{O_2} + 12.48 + 0.78 + 14.04$

$n_{O_2} = 5.75$ mol

Test yourself p: 134

1. methane consumed = In − out = 100 − 40 = 60 mol

   fraction conversion = $\frac{100 - 40}{100} = 0.6$

2. oxygen consumed = 250 − 130 = 120 mol

   Fractional conversion = $\frac{120}{250} = 0.48$

3. $n_i = n_{io} + \Sigma \nu_i \xi$

   CH_4: $40 = 100 - \xi$ $[\xi = 60]$

   O_2: $130 = 250 - 2\xi$

   CO_2: $60 = 0 + \xi$

4. 4 independ molecular species.

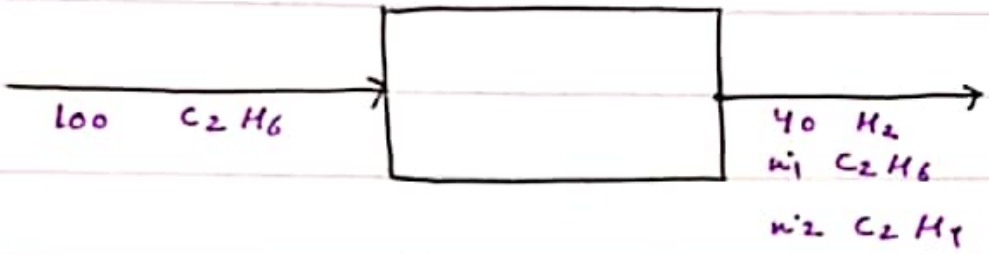
   3 atomic independ.

5. b. Atomic O $2 \times 250 = 130 \times 2 + 2 \times 60 + 120$

   c. molecular O_2 $250 + 0 = 130 + 120$ consumed

   d. water $0 + 120_{\text{generated}} = 120$

   e. Atomic hydrogen $4 \times 100 = 40 \times 4 + 120 \times 2$



$$C_2H_6 \longrightarrow C_2H_4 + H_2$$

- Balance on total mass : In = out
- Balance on C_2H_6, C_2H_4, H_2 : In ≠ out
- Balance on atom C, H : In = out

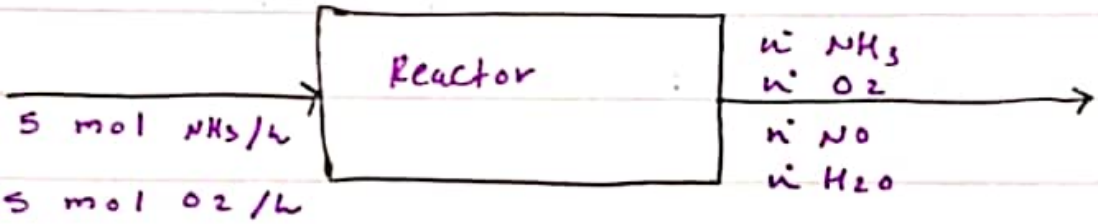
Atoms → In = out

Molecular → In + generation = out + consumption at steady state.

- If no reaction occur → use the DOF method for non reacting systems.
- If reactions occur in the block, you must use DOF for reacting systems.

Example

Ammonia is burned to form oxide. The fractional conversion of O_2 is 0.5. The inlet molar flow rates of NH_3 and O_2 are 5 mol/h. calculate the exit component molar flow rates using : extent of reaction, Atomic balance, molecular balance.



$$4\,NH_3 + 5O_2 \longrightarrow 4\,NO + 6H_2O$$

fractional conversion $= \frac{5 - \dot{n}O_2}{5} = 0.5 \quad \dot{n}O_2 = 2.5$ mol/h

Atomic Species balance:

DoF : + 4 unknowns

− 3 atoms

− 0 non reactive

− 1 relation (fractional conversion)

DOF = 0 ✓

O balance → $2 \times 5 = 2 \times 2.5 + \dot{n}NO + \dot{n}H_2O$

$\dot{n}H_2O = 5 - \dot{n}NO$ —— (1)

N balance : $5 \times 1 = \dot{n}_{NH_3} + \dot{n}_{NO}$

$5 = n_{NH_3} + n_{NO} \rightarrow n_{NH_3} = 5 - n_{NO}$ --- (2)

H balance : $3 \times 5 = 3\dot{n}_{NH_3} + 2\dot{n}_{H_2O}$ ---- (3)

$15 = 3n_{NH_3} + 2(5 - n_{NO})$

$15 = 3n_{NH_3} + 10 - 2n_{NO}$

$15 = 15 - 3n_{NO} + 10 - 2n_{NO}$

$-10 = -5n_{NO}$ $\quad n_{NO} = 2$ mol/h

$\dot{n}_{H_2O} = 5 - n_{NO} = 5 - 2 = 3$ mol/h

$5 = n_{NH_3} + n_{NO}$

$n_{NH_3} = 3$ mol/h

Extent of reaction

DOF : + 4 unknowns

+ 1 reaction

− 4 reactive

− 0 non reactive

− 1 relation

DOF = 0

NH_3 : $\dot{n}_{NH_3} = 5 - 4\xi$ $\quad O_2$: $2 \cdot 5 = 5 - 5\xi$

$\dot{n}_{NH_3} = 3$ mol/h $\quad [\xi = 0.5$ mol/h$]$

NO : $\dot{n}_{NO} = 0 + 4\xi \rightarrow \dot{n}_{NO} = 2$ mol/h

H_2O : $\dot{n}_{H_2O} = 0 + 6\xi \rightarrow \dot{n}_{H_2O} = 3$ mol/h

Molecular balance: In + generation = out + consumption

DOF

+ 4 unknowns

+ 1 reaction

− 4 molecule

− 1 relation

DOF = 0 ✓

NH_3 balance: 5 + 0 = n_{NH_3} + consumption

O_2 balance: 5 + 0 = 2.5 + consumption

Consumption of O_2 = 2.5

$$5 = n_{NH_3} + 2.5\ O_2 \times \frac{4\ NH_3}{5\ O_2}$$

n_{NH_3} = 3 mol/h

NO balance: 0 + generation = n_{NO} + 0

$$2.5\ O_2 \times \frac{4\ NO}{5\ O_2} = n_{NO}$$

n_{NO} = 2 mol/h

H_2O balance: 0 + generation = n_{H_2O} + 0

$$2.5\ O_2 \times \frac{6\ H_2O}{5\ O_2} = n_{H_2O}$$

n_{H_2O} = 3 mol/h

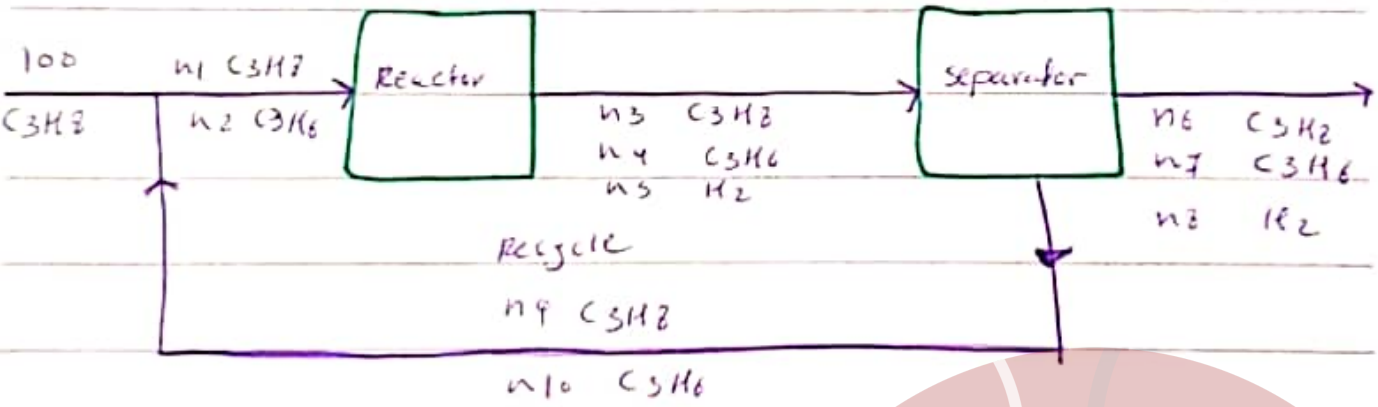
4.7f

overall conversion = $\frac{\text{Input to process} - \text{output from process}}{\text{Input to process}}$

Single-pass conversion = $\frac{\text{Input to reactor} - \text{output from reactor}}{\text{Input to reactor}}$

overall conversion > single pass conversion

4.7-2 (example)



overall conversion → 95 %

$n_6 = 0.555\ \% \times n_3$

$n_{10} = 5\ \% \times n_7$

} relations

DOF on separator

molecular: 8 unknowns + 0 reaction − 3 m species − 2 relation

DOF = 8 − 5 = 3 ∝

Dof overall system

Molecular : + 3 unknowns

+ 1 reaction Dof = 0 ✓

− 3 m species

− 1 relation (95% overall conversion)

Atomic : + 3 unknown

− 2 atoms Dof = 0 ✓

− 1 relation (95%)

Extent of reaction: 3 unknowns

1 reaction

3 m species Dof = 0 ✓

1 relation (95%)

overall conversion = $\frac{\text{In to overall} - \text{out from overall}}{\text{In to overall}}$

$0.95 = \frac{100 - n_6}{100}$ $n_6 = 5$ mol C_3H_8

Molecular species balance In + generation = out + consumption

C_3H_8 : 100 = 5 + consumption → Consumption = 95

C_3H_6 : 0 + generation = out n_7 = generation

$n_7 = 95$ mol C_3H_6

H_2 : 0 + generation = out n_8

Composition of the product Stream?

$n_{total} = n_6 + n_7 + n_8 = 5 + 95 + 95 = 195$ mol

$y_{C_3H_8} = 5/195 = 0.025$

$y_{C_3H_6} = 95/195 = 0.487$ $\quad y_{H_2} = 95/195 = 0.487$

Extent of reaction $\quad n_i = n_{i0} + \nu_i \xi$

$C_3H_8 \rightarrow \quad 5 = 100 - \xi \quad \xi = 95$ mol

$C_3H_6 \rightarrow \quad n_7 = 0 + \xi \quad n_7 = 95$ mol

$H_2 \rightarrow \quad n_8 = 0 + \xi \quad n_8 = 95$ mol

Atomic balance

C balance: $3 \times 100 = 3n_6 + 3n_7$

$300 = 15 + 3n_7 \rightarrow n_7 = 95$ mol

H balance: $8 \times 100 = 2n_8 + 8n_6 + 6n_7$

$800 = 2n_8 + 8 \times 5 + 6 \times 95$

$n_8 = 95$ mol

Note: اذا عندي تفاعل واحد الأسهل اول من طريق Atomic balance ← اكثر من تفاعل ← اذا (extent of reaction)

$n_6 = 0.00555 \times n_3 \longrightarrow n_3 = 900.9 \text{ mol}$

$n_{10} = 0.05\, n_7 \longrightarrow n_{10} = 4.75 \text{ mol}$

Separator system: (no reaction occurs

(In = out لا يحدث تفاعل

H_2 balance: $n_5 = n_8 = 95 \text{ mol}$

C_3H_8 balance: $n_3 = n_6 + n_9 \rightarrow n_9 = 895.9 \text{ mol}$

C_3H_6 balance: $n_9 = n_7 + n_{10} \rightarrow n_{10} = 99.75 \text{ mol}$

$$\frac{\text{moles recycled}}{\text{moles fresh feed}} = ? = \frac{n_9 + n_{10}}{100} = \frac{900.65}{100} = 9.0065$$

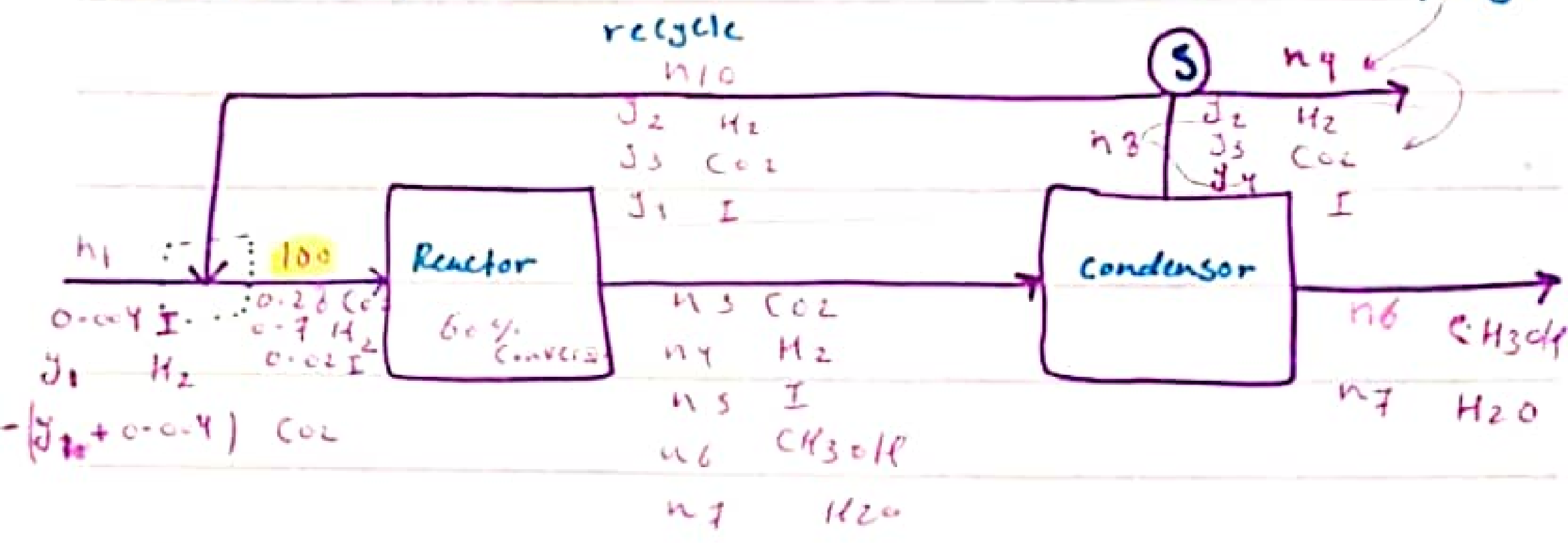
Single-pass conversion ? I need n_1 and n_2

C_3H_8 : $100 + n_9 = n_1 \qquad n_1 = 995.9 \text{ mol}$

C_3H_6 : $0 + n_{10} = n_2 = 4.75 \text{ mol}$

$$\text{Single pass conversion} = \frac{995.9 - 900.9}{995.9} = 0.095$$

Example 4.7-3



Separator : ما بتغير ال composition

و material balance إلها ١ حل.

assume a basis of calculation (100) feed to reactor → ال (composition) نعتمد عليه كل تحسبات

DoF (molecular , extent of reaction)

on reactor: + 5 unknowns + 1 reaction − 5 molecular species

DoF = 6 − 6 = 0 ✓ − 1 relation (60%)

on overall system: + 6 unknowns + 1 reaction − 5 m species

DoF = 7 − 5 = 2 ✗

Extent of reaction $n_i = n_{i0} + \sum \nu \xi$

single-pass conversion of H_2 = $\frac{70 - n_4}{70} = 0.6$

$42 = 70 - n_4 \rightarrow n_4 = 28$ mol/h

Reactor:

H_2 : $28 = 0.7 \times 100 - 3\xi$

$\xi = 14$ mol

CO_2 : $n_3 = 0.28 \times 100 - 14$

$n_3 = 14$ mol

inert → In − out $\quad n_5 = 2$ mol

CH_3OH : $n_6 = 0 + \xi = 14$ mol

H_2O : $n_7 = 0 + \xi = 14$ mol

Condensor:

$n_3 + n_4 + n_5 = n_8 \qquad n_8 = 14 + 28 + 2 = 44$ mol

$y_2 = \frac{n_4}{n_8} = \frac{28}{44} = 0.636$ mol H_2/mol

$y_3 = \frac{n_3}{n_8} = \frac{14}{44} = 0.318$ mol CO_2/mol

$y_4 = 1 - (0.636 + 0.318) = 0.046$ mol I /mol

mixer:

Inert balance: $0.004 n_1 + 0.046 n_{10} = 0.02 \times 100$

$0.04 n_1 + 0.046 n_{10} = 2 \quad (1)$

total balance: $n_1 + n_{10} = 100$

$$n_1 = \frac{2 - 0.045\, n_{10}}{0.004} \qquad \frac{2 - 0.045\, n_{10}}{0.004} + n_{10} = 100$$

$$\frac{2 - 0.045\, n_{10} + 0.004\, n_{10}}{0.004} = 100$$

$$0.4 = 2 - 41 \times 10^{-3}\, n_{10} \qquad n_{10} = 39 \text{ mol}$$

$$n_1 = 61 \text{ mol}$$

Splitter $\quad n_8 = n_9 + n_{10}$

$$44 = n_9 + 39 \qquad n_9 = 5 \text{ mol}$$

Mixer

H_2 balance $\quad 0.636 \times 39 + 61 \times y_1 = 100 \times 0.7$

$$y_1 = 0.74$$

	True value	Assumption
n_0	155 kmol/h	14
n_2	100 × 155/14 = 1107	100
n_1	61 × 155/14 = 675	61
n_9	5 × 155/14 = 55.4	5
n_{10}	39 × 155/14 = 431.8	39

4.8 Combustion reactions

Combustion: rapid reaction of a fuel with oxygen

when a fuel is burned:

- carbon forms CO_2 (complete combustion)
  or CO (partial combustion)
- Hydrogen forms H_2O
- Sulfur forms SO_2
- Nitrogen forms NO when above 1800°C

Composition on wet basis:

Component of mole fractions of a gas that contains water

composition on a dry basis:

Component mole fractions of the same gas without water.

Stack or flue gas:

The product gas that leaves a combustion furnace.

Theoretical oxygen amount of O_2 needed for complete combustion (Stiochodric)

Theoretical air amount of air that contains the theoritical oxygen

$$\text{percent excess air} = \frac{n \text{ air fed} - n \text{ air theoretical}}{n \text{ air theoretical}} \times 100$$

$$= \frac{\text{In } O_2 - \text{theoritical } O_2}{\text{theoretical } O_2}$$

Air in (air feed) = (1 + fractional percent) x theoretical air

O2 in = (1 + fractional percent) x theoritical O2

Material balance on combustion reactors:

- when you draw and label the flowchart, the outlet stream (stack gas) includes:
- unreacted fuel (unless it's completly consumed)
- unreacted oxygen
- water and CO2 (carbon dioxide) and CO carbone monoxide if the combustion is partial (incomplete).
- nitrogen if air is used as the oxygen source, and not pure oxygen.

- calculate the O2 feed rate from a percent excess oxygen or percent excess air (both have the same value)
- If one reaction is involved, all 3 balances methods are convenient (extent of reaction)
- If multiple reactions → Atomic species balance

Example 4-8-1

wet → dry

assume n wet = 100 mol

(افرض basis للي حارته ال composition تبعه)

$n_{N_2} = 60$ mol, $n_{CO_2} = 15$ mol, $n_{O_2} = 10$ mol

$n_{dry} = 60 + 15 + 10 = 85$ mol

$y_{N_2} = \frac{60}{85} = 0.706$ $\quad y_{CO_2} = \frac{15}{85}$ 0.176

$y_{O_2} = \frac{10}{85} = 0.118$

dry → wet

assume basis $ n dry = 100 mol

wet = dry gases + H_2O

100 $\qquad$ n_1

0.93 $\qquad$ 0.07

$n_1 = \frac{100 \times 0.07}{0.93} = 7.527$ mol

$n_{wet} = 100 + n_1 = 100 + 7.527 = 107.527$

composition on weed basis ?

$y = \frac{n}{n_{wet}}$ $\qquad y_{H_2O} = 0.07$ given $\quad y_{N_2} = \frac{65}{107.527}$

$y_{N_2} = 0.604$

$$y_{CO_2} = \frac{14}{107.527} = 0.13$$

$$y_{CO} = \frac{11}{107.527} = 0.102$$

$$y_{O_2} = \frac{10}{107.527} = 0.092$$

Test yourself p:145

1. 21 % O_2 79 % N_2, $79/21 = 3.762$

2. $n_{wet} = 1+1+2 = 4$ $n_{dry} = 1+1 = 2$

dry :

$y_{H_2} = 1/2$ $y_{O_2} = 1/2$

wet :

$y_{H_2} = 1/4$ $y_{O_2} = 1/4$

$y_{H_2O} = 2/4 = 1/2$

3. 0.05 mol H_2O/mol

a. 100 / 5 = 20 fuel = 100

b. 95/100 = 0.95 fuel = dry + H_2O

c. 5 / 95 = 0.052

Example 4.8-2

Complete combustion

$C_4H_{10} + \frac{13}{2} O_2 \longrightarrow 4CO_2 + 5H_2O$

percent excess air = ? $\frac{O_2 \text{ In} - \text{Theoretical } O_2}{\text{Theoretical } O_2}$

1. Find theoretical O_2 (stiochiometric O_2)

based on feed fuel (butane in this example)

Theoretical $O_2 = \frac{100 \times 13/2}{1} = 650$ mol/hr

$= \frac{\text{Fuel In} - \text{Stioch. } O_2}{\text{stoich fuel}}$

- 2 ways to calculate percent excess: (From equation)

1- From air 2 - From oxygen

Theoretical air $= \frac{650}{0.21} = 3095.24$

% excess $= \frac{\text{Air In} - \text{Theoretical air}}{\text{Theoritical air}} \times 100 = \frac{5000 - 3095.24}{3095.24} \times 100$

$= 61.5\ \%$

From oxygen $\longrightarrow$ $0.21 \times 5000 = 1050$ mol/hr : O_2 In

% excess $= \frac{O_2 \text{ In} - \text{theoritical } O_2}{\text{theoritical } O_2} \times 100 = \frac{1050 - 650}{650} = 61.5\%$

4.8 - 3 2 reactions : complete and partial

$C_2H_6 + 7/2\ O_2 \longrightarrow 2CO_2 + 3H_2O$

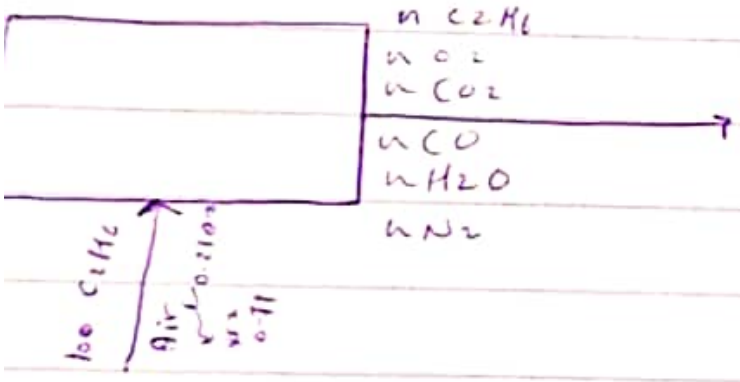
$C_2H_6 + 5/2\ O_2 \longrightarrow 2CO + 3H_2O$

لو بدي احل على atomic بتكفي اعادة اكوي.

لو حل على extent of reaction لازم اعادتين.

Theoretical O_2 ⟵ based on main reaction (الي بدي)

$$\text{Theoretical } O_2 = \frac{\text{fuel} \times \text{stoich } O_2}{\text{stoic fuel}} = \frac{100 \times 7/2}{1} = 350 \text{ mol}$$



$$\frac{25\%CO}{75\%CO_2} = \frac{1}{3}$$

$$\frac{n_{CO_2}}{n_{CO}} = 3$$

O_2 In = (fractional percent + 1) × theoretical O_2

= 525 mol

$$N_2 \text{ In} = \frac{O_2 \text{ In}}{0.21} \times 0.79 = \frac{525}{0.21} \times 0.79 = 1975 \text{ mol}$$

$$\text{conversion of ethane} = \frac{100 - n_{C_2H_6}}{100} = 0.9$$

$$90 = 100 - n_{C_2H_6} \qquad n_{C_2H_6} = 10 \text{ mol}$$

n_{N_2} out = 1975 because 1% is inert

extent of reaction method: $n_i = n_{i0} + \Sigma \nu \xi$

$C_2H_6 \rightarrow$ $10 = 100 - \xi_1 - \xi_2$ ---- (1)

$CO_2 \rightarrow$ $n_{CO_2} = 0 + 2\xi_1$ ---- (2)

$CO \rightarrow$ $n_{CO} = 0 + 2\xi_2$ ---- (3)

$\frac{n_{CO_2}}{n_{CO}} = 3$ --- (*) $\quad n_{CO_2} = 3n_{CO}$ -- (4)

$3n_{CO} = 2\xi_1$ $\quad n_{CO} = 2\xi_2$

$-90 = -\frac{3n_{CO}}{2} - \xi_2$ $\quad \xi_2 = \frac{n_{CO}}{2}$

$-90 = -\frac{3n_{CO} - n_{CO}}{2}$ $\rightarrow -180 = -4n_{CO}$

$n_{CO} = 45$ mol

$n_{CO} = 2\xi_2$ $\quad 45 = 2\xi_2 \rightarrow \xi_2 = 22.5$ mol

$10 = 100 - \xi_1 - 22.5 \rightarrow \xi_1 = 67.5$ mol

$n_{CO_2} = 2\xi_1 = 2(67.5) = 135$ mol

$O_2 \rightarrow$ $n_{O_2} = 525 - 7/2\,\xi_1 - 3/2\,\xi_2$

$n_{O_2} = 232.5$ mol

$H_2O \rightarrow$ $n_{H_2O} = 0 + 3\xi_1 + 3\xi_2$

$n_{H_2O} = 270$ mol

molar composition on dry basis ? (without H_2O)

$n_{dry} = n_{C_2H_6} + n_{O_2} + n_{N_2} + n_{CO_2} + n_{CO} =$

$n_{dry} = 2375$ mol

$y_{C_2H_6} = \frac{10}{2375} = 0.0042$ | $y_{O_2} = \frac{232.5}{2375} = 0.097$

$y_{N_2} = \frac{1975}{2375} = 0.832$ $y_{CO_2} = \frac{135}{2375} = 0.056$

$y_{CO} = \frac{45}{2375} = 0.019$

ratio of mol water to dry gas $\rightarrow n_6/n_{dry}$

$\frac{270}{2375} = 0.113$

(Atomic species balance)

C balance : $100 \times 2 = 10 \times 2 + n_{CO_2} + n_{CO}$

$200 = 20 + n_{CO_2} + n_{CO}$

$[n_{CO_2} = 3n_{CO}]$ $180 = 3n_{CO} + n_{CO}$

$180 = 4\, n_{CO}$

$n_{CO} = 45$ mol

$n_{CO_2} = 135$ mol

H_2 balance: $6 \times 100 = 6 \times 10 + 2n_{H_2O}$

$$n_{H_2O} = \frac{600 - 60}{2} = 270 \text{ mol}$$

O balance: $2 \times 525 = 2n_{O_2} + 2n_{CO_2} + n_{CO} + n_{H_2O}$

$1050 = 2n_{O_2} + 270 + 45 + 270$

$n_{O_2} = 232.5$ mol

CH: 5 Single-phase system

- Solid and Liquid densities are independent of temperature and pressure so they are incompressible.

Two ways to calculate the density of a mixture:

1. assuming volumes are additive.

$$\frac{1}{\bar{\rho}} = \sum_{i=1}^{n} x_i / \rho_i$$

best for ideal mixtures

2. $\bar{\rho} = \sum_{i=1}^{n} x_i \rho_i$ No general rule

Test your self p: 190

1. $v^{\cdot} = m^{\cdot} / \rho = 255\ g/s \times \frac{cm^3}{1\ g} = 255\ cm^3/s$

$m^{\cdot}$ stays constant, but $v^{\cdot}$ increases a little.

2. Because pressure varies with temperature, the difference will be small.

3. $\frac{1}{\bar{\rho}} = \frac{V_{total}}{m_{total}}$

$$1/\bar{\rho} = \frac{m_1}{m_{total}\,\rho_1} + \frac{m_2}{m_{total}\,\rho_2} + \frac{m_w}{m_{total}\,\rho_w}$$

$$1/\rho = \frac{x_1}{\rho_1} + \frac{x_2}{\rho_2} + \frac{x_w}{\rho_w}$$

Example 5.1 - 1

density of H_2SO_4 solution = ?

50 % H_2SO_4 50 % water

1. Looking a tabulated value → $\rho = 1.3951\ g/cm^3$

2. assuming additivity of the components:

$\rho_{H_2O} = 0.998\ g/cm^3$ $\rho_{H_2SO_4} = 1.834\ g/cm^3$

$x_{H_2O} = \frac{50}{100} = 0.5$ $x_{H_2SO_4} = 0.5$

$1/\bar{\rho} = 0.5/0.998 + 0.5/1.834 = 1/0.774 = 1.292$

$$\text{error\%} = \frac{x_m - x_{true}}{x_{True}} \times 100 = \frac{.292 - 1.3951}{1.3951} \times 100$$

7.3 ← الخطأ $= -7.3\ \%$

لو حل القانون الثاني

$p = \Sigma x_i p_i = 0.5 \times 0.998 + 0.5 \times 1.834$

$= 1.42$

(this equation is better).

لأنه أقرب للقيمة الحقيقية.

5.2 IDEAL GAS

- gas properties are usually strong affected by temperature and pressure, unlike liquids and solids.

Ideal gas equation of state: "perfect gas"

$PV = nRT$ or $P\dot{V} = \dot{n}RT$

$\rho = \frac{P \bar{M}}{RT}$ (to calculate density of ideal gas)

P: absolute pressure of gas

V: volume of gas

n: number of moles for gas

R: gas constant

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

$\bar{M} = \Sigma y_i M_i$

mixture اذا عندي

بحسب ال $\bar{M}$ بحسب ال ... وأعوض بكتب الكتلة المولية ال

$R = 8.314\ J/mol.K = 0.082\ L.atm/mol.K$

$= 10.73\ ft^3.psia/lb\ mol.R°$

T: absolute temperature of the gas.

(kelvin or Rankine)

Gas is ideal when:

- Low pressure (below 1 atm) and high temperature (above 0 C°).

- 1 mol of ideal gas at 0C° and 1atm (STP conditions) is 22.415 Liters

Conversion from standard conditions:

(To avoid converting the units)

$$\frac{P V}{P_s V_s} = n \frac{T}{T_s}$$

P and T should be absolute → P in atm, T in K

P_s = 1 atm

T_s = 0C° = 273 K

$v_s = 22.4 \frac{m^3}{kmol} = 22.4 \frac{L}{mol} = 359 \frac{ft^3}{lbmol}$

SCM: Standard cubic meters m^3 (STP) at 0C°, 1atm

SCF: Standard cubic feet ft^3 (STP) at 0C°, 1atm

- volumetric flow rate of 18.2 SCMH means (Standard / cubic / meter / hour)

18.2 m^3/h at 0C°, 1atm

V° of 18.2 SCFM → 18.2 ft^3/min at 0C°, 1atm

(cubic ft per min)

5.2 c Ideal gas mixtures

Partial pressure of A (PA) : pressure that would be exerted by (nA) moles of A alone in the same total volume at the same temperature.

Dalton's Law:

$$P_A = J_A P$$

J_A : mole fraction of A

P: total pressure

- partial pressure of a component in an ideal gas mixture is the mole fraction of that component times the total pressure.

$$\underbrace{P_A + P_B + P_C}_{\text{مجموع الضغوط الجزيئية}} = (J_A + J_B + J_C) P = P$$

total pressure الكلي الضغط يساوي مجموع الضغوط الجزيئية.

- pure Component Volume of A (V_A) : the volume that would be occupied by (nA) moles of A alone at the total pressure and the temperature of the mixture.

Amagat's Law:

$$V = V_A + V_B + V_C + \dots$$

The volume fraction of a substance in an ideal gas mixture equals the mole fraction of this substance.

$$\frac{V_A}{V_{total}} = \frac{n_A}{n_{total}} = y_A$$

$\frac{V_A}{V_{total}}$ → volume fraction

y_A → mole fraction

Example 5.2-1

N_2 : 100 g $t = 23c$ $P_{gauge} = 3$ psi

1. Volume in L ? (ideal)

$PV = nRT$

$n = \frac{m}{M.W} = \frac{100}{28} = 3.57$ mol

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

$3 \text{ psi} + 1 \text{ atm} \cdot \frac{14.7 \text{ psi}}{\text{atm}} = 17.7$ psi absolute

$17.7 \text{ psi} \cdot \frac{1 \text{ atm}}{14.7 \text{ psi}} =$ Pabs in atm $= \frac{17.7}{14.7} = 1.2$ atm

in pascal $= \frac{1.2 \text{ atm}}{} \cdot \frac{1 \text{ ... Pa}}{1 \text{ atm}}$

$P_{pascal} = 121590$

12159 · $PV = nRT$ نستعمل pressure (باسكال)

$V = 3.57 \times (8.314) \times (23 + 273.15)$

$V = 0.072 \text{ m}^3 \times \frac{1000 \text{ L}}{\text{m}^3}$ $1 \text{ m}^3 = 1000$ L

$V = 72$ L

$1.2 \; V = 3.57 \times 0.082 \times (273 + 23)$

$V = 72$ L

2. N_2 is diatomic gas so $\tilde{V}$ ideal should be > 5 L / mol

$\tilde{V} = \frac{RT}{P} = \frac{V}{n} = \frac{72 \text{ L}}{3.57 \text{ mol}}$ $20.16 > 5$

error will be less than 1 %.

5.2-2 Example

360 C° 3 atm absolute $\dot{m} = 1100$ kg/h

$\dot{V} = ?$ from Standard conditions → 1 atm, 0C°

$P\tilde{V} = RT$ ---- ① $PV = nRT$ ---- ②

$$\frac{PV}{P_s \tilde{V}_s} = \frac{nRT}{RT_s} \qquad \frac{PV}{P_s V_s^{\circ}} = \frac{nT}{T_s}$$

$$\dot{n} = \frac{\dot{m}}{M.w} = 1100 \text{ kg/h} \times \frac{1 \text{ kmol}}{58.1 \text{ kg}} = 18.93 \text{ kmol/h}$$

$$\frac{3 \times V}{1 \times 22.4 \frac{m^3}{kmol}} = 18.93 \frac{kmol}{h} \times \frac{633 K}{273 K}$$

$$V = 327.7 \text{ m}^3/\text{h}$$

5.2-3

Air

70°F

1 atm

10 ft³

$P_1 V_1 = n R T_1$

heat

610°F

2.5 atm

$V_2 = ?$

$P_2 V_2 = n R T_2$

(same number of moles because it's the same gas)

$$\frac{P_2 V_2}{P_1 V_1} = \frac{T_2}{T_1}$$

$$P_2 V_2 T_1 = P_1 V_1 T_2$$

$$V_2 = \frac{P_1 T_2 V_1}{P_2 T_1}$$

$$V_2 = \frac{1 \text{ atm} \times 1070 R^\circ}{2.5 \text{ atm} \times 530 R^\circ} \times 10 \text{ ft}^3 = 8.08 \text{ ft}^3$$

T and P should be absolute

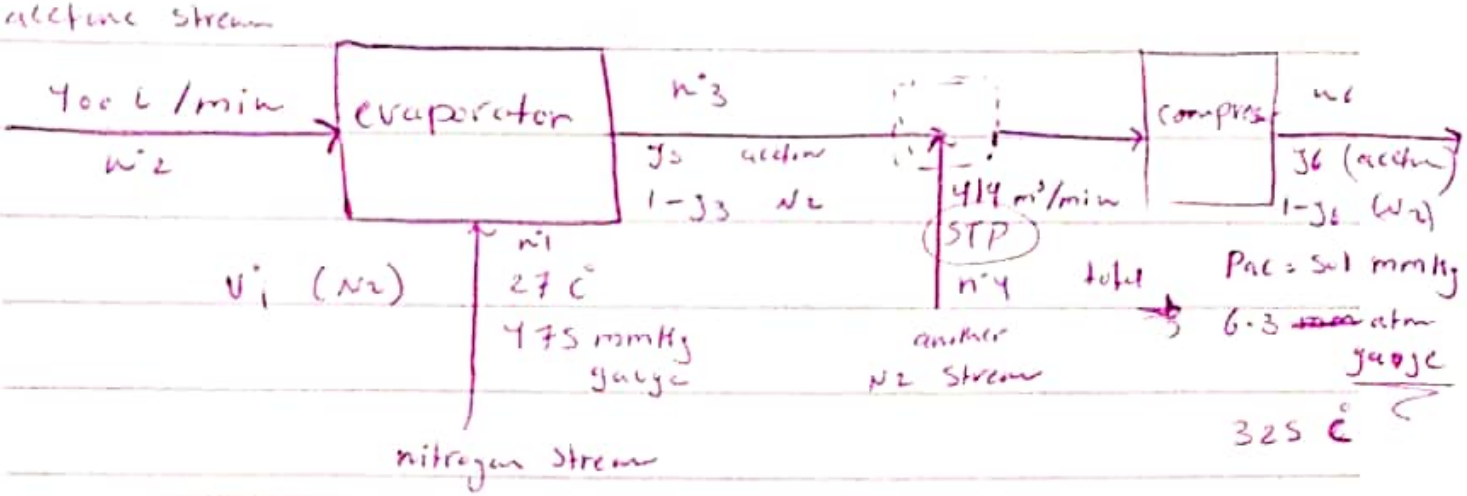
$T_R = T_F + 460 = 610 + 460 = 1070 R^\circ \ (T_2)$

$T_1 = 70 + 460 = 530 \ R^\circ$

T → K or R°

P → absolut pressur

Example 5.2-5



$P_{atm} = 763$ mmHg

DOF on overall

unknowns: ($\dot{n}_2$, V_1, ω_1, $\dot{n}_4$, y_6, $\dot{n}_5$) 6 unknowns

species (material balance): (acetone, N_2) 2

relations: ($\dot{n}_2, V_2$ – ($\dot{n}_1 V_1$) – ($\dot{n}_4 V_4$) – (dalton's Law) → partial pressure with y_6)

4 relations

$\dot{n}_2$ = ? Find $\dot{n}_2$ from ρ and $\dot{V}_2$

$$\dot{m}_2 = \rho \times \dot{V}_2 = 0.741 \frac{g}{cm^3} \times \frac{400 L}{min} \times \frac{10^6 cm^3}{1000 L} = 316.4 \times 10^3 \ g/min$$

$$\dot{n}_2 = \dot{m}_2 / M.w = 316.4 \times 10^3 \frac{g}{min} \times \frac{mol}{58 g} = 5.455 \times 10^3 \ mol/min$$

Stream 4 at STP so 1 gmol → 22.4 $\frac{L}{mol}$ = 22.4 $\frac{m^3}{kmol}$

$$\dot{n}_4 = 419 \frac{m^3}{min} \times \frac{1 kmol}{22.415 m^3} = 18.6 \frac{kmol}{min} \times \frac{10^3 mol}{1 kmol} = 18.6 \times 10^3 \ mol/min$$

y_6 → (dalton's Law) $P_{acetone} = y_6 P_{total}$

absolute

Sol mmHg = $y_6 \times 5.569 \times 10^3$

$y_6 = 0.09$ mol acetone/mol

Ptotal = 6.3 atm gage

Pabs = 1 atm + 6.3 atm

$= 7.3 \text{ atm} \cdot \frac{763 \text{ mmHg}}{1 \text{ atm}}$

$P_{abs\,(total)} = 5.569 \times 10^3$ mmHg

Starting material balance:

acetone balance:

$\dot{n}_2 = y_6 \dot{n}_6$

$5.455 \times 10^3 = 0.09 \times \dot{n}_6$ $\quad \dot{n}_6 = 60.61 \times 10^3$ mol/min

Total balance:

$\dot{n}_2 + \dot{n}_1 + \dot{n}_4 = \dot{n}_6$

$5.455 \times 10^3 + \dot{n}_1 + 18.6 \times 10^3 = 60.61 \times 10^3$

$\dot{n}_1 = 36555$ mol/min

$V_1 = ?$ $\quad PV = nRT$

475 mmHg gage + 1 atm $\cdot \frac{763 \text{ mmHg}}{\text{atm}} = 1238$ mmHg abs

$n_1 = 36555$ mol/min

$T = 27 + 273 = 300$ K $\quad R = 62.36$ L mmHg/(mol·K)

$V = \frac{36555 \times 62.36}{1238} \times 300 = 552.4 \times 10^3$ L/min

$552.4 \times 10^3 \frac{L}{min} \times \frac{1 \text{ m}^3}{10^3 \text{ L}} = 552.4$ L/min

5.3 equations of state for non-ideal gases

- **Critical temperature**: The highest temperature at which a species can coexist in two phases and the corresponding pressure is the critical pressure.

- **critical state**: substance at T_c and p_c.

Difference between gas and vapor ?

- vaper: gaseous species below it's critical Temperature while gas is a species above it's critical temperature and a low pressure
- vapor can be condensed, while gas can't.

- **supercritical fluids** substance at temperature above T_c and pressure above P_c.

Test yourself 200

1. below T_c → (vapor)
2. $p_b > p_a$ $P_{va} < P_{vb}$ $P_{la} > P_{lb}$

3. no condensate because it's gas (above T_c) and Low P

find condition ⟶ supercritical fluid (above T_c and P_c).

Example 5-3-1

$V = 3\ L$ — $n = 2\ mol\ N_2$

$T = -150.8\ C^\circ$

$P = ?$ using ideal gas and then virial equation

percentage error = ?

$T_K = -150.8 + 273.15 = 122.35$

$PV = nRT$

$$P = \frac{2\ mol \times 0.082 \times 122.35\ K}{3\ L} = 6.69\ atm$$

virial equation $\frac{PV^-}{RT} = 1 + \frac{B}{V^-}$

$B_0 = 0.083 - \frac{0.422}{(T_r)^{1.6}}$, $T_r = T / (T_c)$ (from B.1)

$T_r = 122.35\ K / 126.2\ K$

$T_r = 0.969$

$B_0 = -0.36$

$B_1 = 0.139 - \frac{0.172}{T_r^{4.2}}$

$B_1 = -0.057$

$B = \frac{RT_c}{P_c}(B^0 + \omega B^1)$

from pitzer table

$$B = \frac{0.082 \left(\frac{\text{L atm}}{\text{mol K}}\right) 126.2\ \text{K}}{33.5\ \text{atm}} \left(-0.36 + 0.04\,x - 0.037\right)$$

$$= -0.112 \quad \text{L/mol}$$

$$\frac{PV^{\sim}}{RT} = 1 + \frac{B}{V^{\sim}} \qquad V^{\sim} = \frac{V}{\text{mol}} = \frac{3\,\text{L}}{2\,\text{mol}} = 1.5 \ \text{L/mol}$$

$$\frac{P \times 1.5\ \text{L/mol}}{0.082 \times 122.35\ \text{K}} = 1 + \frac{-0.112\ \text{L}}{1.5\ \text{L/mol}}\ \text{mol}$$

$\frac{\text{L atm}}{\text{mol K}}$

$$0.1495\,P = 0.9253$$

$$P = 6.19 \ \text{atm}$$

$$\text{error \%} = \frac{P_{ideal} - P_{virial}}{P_{ideal}} \times 100\ \%$$

$$= 7.1 \ \%$$

5.3b virial equation of state

$$\frac{P\,v^{\sim}}{RT} = 1 + \frac{B}{v^{\sim}} \qquad , \; v^{\sim} = \frac{V}{n} = \left(L/m\right.$$

$$B = \frac{RT_c}{P_c}\left(B_0 + \omega B_1\right)$$

$$B_0 = 0.083 - \frac{0.422}{T_r^{1.6}}$$

$$B_1 = 0.139 - \frac{0.172}{T_r^{4.2}}$$

$$T_r = T / T_c$$

- T given in question
- T_c and P_c from table (B.1).
- ω from pitzer Acentric " Each Compound has an Acentric factor "

Note:

- Solution for P is straight forward. but If $v^{\sim}$ is to be determined, the equation can be rearranged into a quadratic and solved using quadratic formula:

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

one of the 2 answers is true → estimate $\tilde{v}$ from the ideal gas equation of state and choose the closest value.

$[PV = nRT]$

5.3c Cubic equation of state

- van der Waals

$$P = \frac{RT}{\tilde{v} - b} - \frac{a}{\tilde{v}^2}$$

$$a = \frac{27 R^2 T_c^2}{64 P_c} \qquad b = \frac{R T_c}{8 P_c}$$

$\tilde{v} = \frac{V}{n \text{ (mol)}}$ T_c and p_c from B.1 table

- Redlich-Kwong, Soave-Redlich-Kwong (SRK) and Peng-Robinson

$$P = \frac{RT}{\tilde{v} - b} - \frac{\alpha a}{\tilde{v}(\tilde{v} + b)}$$

$$a = 0.42747 \frac{(RT_c)^2}{P_c} \qquad b = 0.08664 \frac{RT_c}{P_c}$$

$$m = 0.48508 + 1.5517 \omega - 0.1561 \omega^2$$

ω from Acentric factor table

$$T_r = T / T_c$$

$$\alpha = \left[1 + m \left(1 - \sqrt{T_r} \right) \right]^2$$

T → given in question

T_c → table B.1

5.4 Compressibility factor equation of State

$$P\tilde{V} = ZRT \qquad \tilde{V} = \frac{V}{n(mols)}$$

- determin Z and the substitute it.

Example 5.4-1

50 m^3/h of CH_4

40 bar (absolute)

300 K

Z = ? $\dot{m}$ = ? Z = 0.934

$$\frac{50\ m^3}{h} \times \frac{1000\ L}{1\ m^3}$$

$V = 50 \times 10^3\ L$

$P\tilde{V} = ZRT \Rightarrow PV = ZnRT$

$$39.4 \times 50 \times 10^3 = 0.934 \times 0.082 \times 300 \times n$$

$$40\ bar \times \frac{1\ atm}{1.01325\ bar}$$

$n = 85.7 \times 10^3\ mol/h$

$P_{abs} = 39.4\ atm$

$m = n \times M.w$

$= 85.7 \times 10^3 \frac{mol}{h} \times 16.04\ g/mol$

$= 1374 \times 10^3\ g/h = 1374\ kg/h$

To estimate z from the chart:

1. calculate reduced temperature T_r and reduced pressure p_r

$T_r = T / T_c$ $\qquad$ $p_r = P / P_c$

2. look up the valve of z on generalized Compressibilty chart which plot z versus pr for valves of T_r.

$$v_r \text{ ideal} = \frac{P_c v}{R T_c}$$

If the gas is hydrogen (H_2) or helium(He) determine the critical constnt from:

$T_c' = T_c + 8\ K$

$p_c' = P_c + 8\ atm$

Example 5.4 – 2

100 mol N_2 $\qquad \tilde{v} = \frac{5\ L}{100\ mol} = 0.05\ L/mol$

5 L :

$-20.6\ C^\circ \longrightarrow 252.4\ K$

estimate $P = ?$

$P\tilde{v} = zRT \qquad Pv = nzRT$

$T_r = T / T_c = 252.4\ K / 126.2\ K = 2$

B.1

$P_c = 33.5\ atm$

$v_{ideal} = \frac{\tilde{v} P_c}{R T_c} = \frac{0.05\ L \times 33.5\ atm}{mol \cdot 0.082 \frac{L \cdot atm}{mol \cdot K} \times 126.2\ K} = 0.162$

$z = ?$ (From the chart) $\longrightarrow z = 1.8$

$P\tilde{v} = zRT \qquad P = \frac{1.8 \times 0.082 \times 252.4}{0.05} = 745\ atm$

5.4c Non ideal gas mixtures

If I have a gas contains: methane, CO_2 and N_2 → (Kay's rule)

estimates pseudocritical properties of mixtures as simple averages of pure component critical constants.

Pseudocritical temperature: $T_c' = y_A T_{cA} + y_B T_{cB}$

$$T_c' = \sum y_i T_{ci}$$

Pseudocritical pressure: $P_c' = y_A P_{cA} + y_B P_{cB}$

Pseudroreduced T: $T_r' = T / T_c'$

Pseudroreduced P: $P_r' = P / P_c'$

Example 5.4-3

0.75 H_2 0.25 N_2 | $P = 800$ atm

Estimate specific volume = ? $\tilde{v}$ = ? | $-70\,C^\circ \rightarrow 203.15\,K$

$$P\tilde{v} = ZRT$$

$$T_r' = T / T_c' \qquad T_c' = \sum y_i T_{ci}$$

$$P_r' = P / P_c'$$

$T_c' H_2 = 33.8 + 8\ K = 41.8\ K$

$P_c H_2 = 12.8 + 8\ atm = 20.8\ atm$

$T_c N_2 = 126.2$

$P_c N_2 = 33.5$

$T_c' = 0.75 \times 41.8 + 0.25 \times 126.2 = 62.9\ K$

$P_c' = 0.75 \times 20.8 + 0.25 \times 33.5 = 23.98\ atm$

$T_r' = T / T_c' = 203.15 / 62.9 = 3.23\ K$

$P_r' = P / P_c' = 800 / 23.98 = 33.4\ atm$

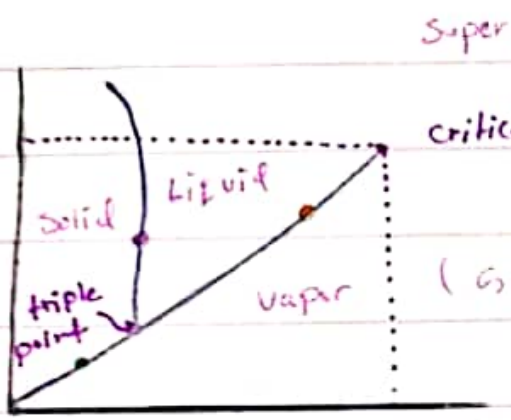
Z_m ← (From Chart) $Z_m = 1.7$

$PV^{\sim} = Z_m RT$

$V^{\sim} = \dfrac{1.7 \times 0.08206 \times 203.15\ K}{800\ atm} = 0.035 \dfrac{L}{mol}$ $\dfrac{L\ atm}{mol\ K}$

6-1 Single Component phase equilibrium.

Phase diagram is a plot of one system variable against another that shows the conditions at which the substance exists as a solid, liquid, gas.



no Condensation ; Supercritical fluid ← critical point is not occurs.

- Above critical point → gas
- Triple point: it's the point at which solid, liquid and vapor phases can all coexist.
- If (T, P) falls on Liquid-vapor equilibrium then P is the vapor pressure of the substance at temperature T and T is the boiling point of this substance at pressure P.

- If (T, p) falls on the solid-liquid equilibrium curve, then T is the melting point (if from solid to liquid) or freezing point (if from liquid to solid) at pressure p.

- If (T, p) falls on the solid-vapor equilibrium then p is the vapor pressure of the solid at temperature T, and T is the sublimation point at pressure p.

Note:

The boiling point of a substance at $p = 1$ atm is the normal boiling point of that substance.

Test yourself P: 243

1. Sublimation point → (solid - vapor) -5 °C

2. at -56.1 °C and 5.112 atm.

3. Solid - vapor equilibrium, solid only when temperature is raised → vapor

4. 1 atm for solid, 9.9 atm for liquid.

5. -78.5 °C, -56.6 °C, -40 °C

6.1 b estimation of vapor pressures

Volatility: is the degree to which the species tends to transfer from the liquid or solid state to the vapor state.

high volatility → vapor pressure

low volatility → condensed phase (Liquid - Solid)

Chapeyron equation

$$\frac{dp^*}{dT} = \frac{\Delta H_v^\sim}{T(v_j - v_i)}$$

p^* : vapor pressure of pure substance.

T : absolute temperature

v_j : specific molar volume for gases (volum/moles).

v_i : specific molar volume for liquid.

$\Delta H_v^\sim$: latent of heat vaporization, energy required to vaporize 1 mole of the liquid.

at low pressures, the specific volume of the liquid is negligible → $(v_g^\sim - v_i^\sim \simeq v_g^\sim)$

applying the ideal gas equation:

$$\frac{d[\ln p^*]}{d(1/T)} = \frac{-\Delta H_v^\sim}{R}$$

Clausius - Clapeyron equation

$$\ln P^* = \frac{-\Delta H_v^*}{RT} + B$$

- B is a const. that varies from one substance to another.

Example 6.1-1 p: 244

calc. heat of vaporization $\Delta H_v^* = ?$

parameter B = ? estimate P^* at 42.2 °C

$$\ln P^* = \frac{-\Delta H_v}{RT} + B$$

$y = mx + b$

$y \rightarrow \ln P^*$ $\quad x \rightarrow 1/T$

Slope $\rightarrow -\Delta H_v^*/R$ $\quad$ intercept $\rightarrow B$

1. find slope

$$\text{slope} = -\Delta H_v^*/R = \frac{\Delta y}{\Delta x} = \frac{\ln(60/10)}{\frac{1}{288.55} - \frac{1}{280.45}} = -4211$$

2. find intercept

$P_2 = 60$ mmHg

$T_2 = 288.55$ K

$$B = \ln P_2^* + \frac{\Delta H_v^*}{R T_2}$$

$$\ln(60) + \frac{4211}{288.5} = 18.69$$

3. p^* at $42.2^\circ = 315.35\ K$

$$\ln p^* = -\frac{\Delta H_v^*}{RT} + B$$

$$= \frac{-4211}{316.35} + 18.69$$

$$\ln p^* = 5.334 \quad | \quad p^* = e^{5.334} = 207\ mmHg$$

heat of vaporization

$$-\frac{\Delta H_v^*}{R} \times R = 4211\ K \times \frac{8.314\ J}{mol \cdot K}$$

$$= 3.5 \times 10^4\ J/mol$$

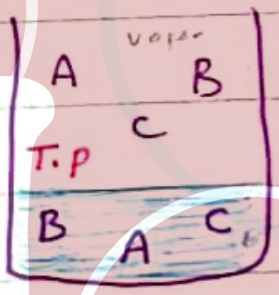
Antoine equation

$$\log_{10} P^* = A - \frac{B}{T + C}$$

values of A, B and C are listed in Table B.4 (T in C° and P^* in mmHg)

6.2 the gibbs phase rule.

when 2 phases are brought into contact with each other, species evaporate, condense, dissolve or precipitate until a state of equilibrium is reached which: temperatures and pressures of both phases are the same and the composition of each phase doesn't change with time.



- we have a vessel containing A, B, C in 2 different phases (Liquid, vapor)

Changes happen in this system like evaporation $C_L \rightarrow C_V$

Condensation $B_g \rightarrow B_L$ or precipitation (becomes solid), dissolving (Solid → Liquid)

To describe this system:

- The system temperature and pressure.
- Masses of each phase
- 2 masses or mole fractions for each phase.

Variables describing the process system:

1. Extensive variables : depends on the size of the system ex, mass and mole fractions, number of moles and molar flow rate, volume and volumetric flow rate
2. Intensive variables : Independ of the system size Temperature, pressure, density, specific volume, mass and mole fractions.

Gibbs phase rule

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

C : number of chemical species

Π : number of phases in a system at equilibrium.

in the previous example :

$$DF = 2 + 3 - 2 = 3$$

Example 6.2-1

1. pure liquid water

$C = 1$ (H_2O) $\quad \pi = 1$ "liquid"

$DF = 2 + 1 - 1 = 2$

2. mixture of liquid, solid, vapor water

$C = 1$ (H_2O) $\quad \pi = 3$ "liquid - solid - vapor"

$DF = 2 + 1 - 3 = 0$

3. vapor - liquid mixture of acetone and methyl ethyl ketone

$C = 2 \quad \pi = 2$

$DF = 2 + 2 - 2 = 2$

Test yourself p: 249

1. extensive variables: depends on the size of the system

Like: number of moles, molar flow rate.

Intensive variables: Independent of the system size

Like: temperature and pressure.

$DF = 2 + C - \pi$

2.

a. $C = 2$ (Na^+, Cl^-) $\pi = 2$ (Solid, Liquid)

$DF = 2 + 2 - 2 = 2$

b. Humid : water + dry air

$C = 2$ $\pi = 2$ (vapor, liquid)

$DF = 2 + 2 - 2 = 2$

c. $C = 4$ $\pi = 2$ (vapor, liquid)

$DF = 2 + 4 - 2 = 4$

d. $C = 3$ $\pi = 1$

equ. reaction = 1

$DF = 2 + 3 - 1 - 1 = 3$

6.3

At equilibrium : the partial pressure of the gas equals the vapor pressure of pure component at the system temperature.

$$p_i = p_i^*(T)$$

partial ↙

Raoults Law

single Condensable species

- when $P_i = P_i^*$ in a single condensable component, any attempt to increase P_i will lead to condensation

- A vapor present in gas less than it's saturation amount ⟶ (super heated vapor)

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

So to achieve condensation in a system containing a super heated vapor one or more of the variables most be changed :

- increasing the pressure at constant temperature.
- decreasing temperature at constant pressure.

"يا بتزيد الضغط او بتقلل الحرارة."

- If the superheated vapor is cooled (decreasing T) at constant pressure, the temperature at which the vapor becomes saturated (at equilibrium) "$P_i = P_i^*$" is referred to as the dew point.

$$P_i = y_i P_i = P_i^* (T_{dp})$$

Degrees of superheat = Temperature - dew point

Evaporation

The temperature at which $P^* = P$ is the boiling point of the Liquid at the given pressure.

Test yourself p: 253

1. yes because it's at equilibrium , yes because

$$P_i = P_i^*(T)$$

2. a. $P_i = y_i P = P_i^*(T)$

Partial P of acetone = 200 mmHg

b. total pressure = 960 mmHg

acetone — Air

79% N_2 21% O_2

$P_{total} = P_{acetone} + P_{air}$

$960 = 200 + P_{air}$

partial pressure of air = 760 mmHg $P_{N_2} = y_{N_2} P_{total\,(air)}$

$y_{N_2} \times P = P_{N_2}$

$760 \times 0.79 = 600.4$ $P_{N_2} = 600.4$ mm

c. $P_{acetone} = P_{acetone}$

$960\ y = 200$

$y = 0.208$ mol acetone / mol

at boiling point $P^*_{(T)} = P$

3.

(a) Dew point: temperature at which $P = P^*(T_{dp})$

partial pressure equals the vapor pressure which the gas becomes saturated.

$T_o > T_{dp}$ ⟶ Superheated vapor (سخن بزیادة بخار)

$T_o = T_{dp}$ ⟶ Saturated (اول ده شان P یبقد)

$y_i = P^*(T) / P_{total}$ $\quad P_i = y_i P = P^*(T)$

(i) nothing changes

(ii) P^* will decrease which will lead to

$y_i P > P^*(T)$

so y_i will decrease by Condensation ⟵

"because P_{total} is constant" (Equilibrium الاتزان بيحاول يوصل)

(iii) we will decrease y_i by Condensation to reach equilibrium because the temperature is constant

(iv) expansions → (↓P) $y_i P < P^*(T)$

nothing will change and will'nt condensate.

c. $y_i P = P^*(T)$ search for T when

$$P_{H_2O} = P^*_{H_2O}(T)$$

d. degree of superheat = Temperature − dew point [of the system]

$T_{dp} = T_o - T$ of superheat

then applying raouls rule

$$P y_{H_2O} = P^*(T_{dp})$$

Example 6.3-1

at equilibrium → $y_i P = P^*(T)$

partial pressure equals vapor pressure

→ raoult's law: $y \times 760 = P^*(75°)$ → from table B-3

$y\ 760 = 289$

$y = 0.38$ mol H_2O / mol

$1 - y = 0.62$ mol dry / mol

6.3-2

1.

$J = 0.1 \quad P_{total} = 5260 \text{ mmHg}$

$P_{H_2O} = 0.1 \times 5260 = 526 \text{ mmHg}$

$P^*_{H_2O}(100^\circ C) = 760 \text{ mmHg}$

$P^*_{H_2O} > P_{H_2O}$ so it's superheated and we need to cool it by decreasing T $\rightarrow$

$P_{H_2O} = J P_{total} = P^*_{H_2O}(T) = 526 \text{ mmHg}$

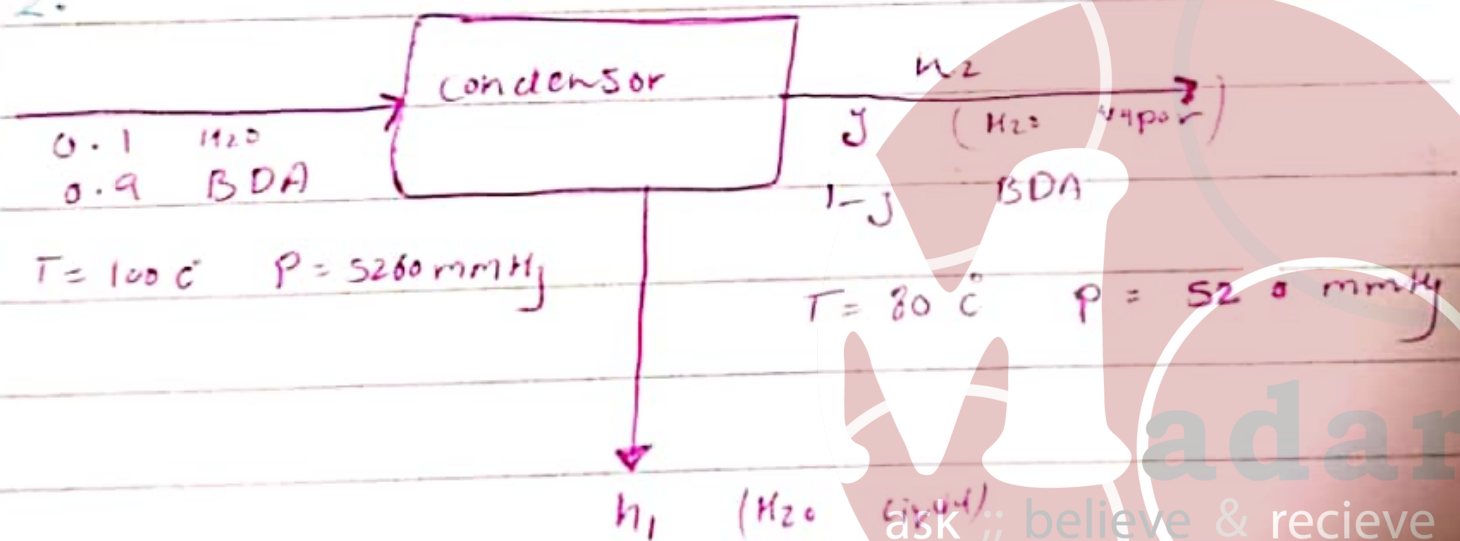
From table B.3 search for T at 526 mmHg

$T_{dp} = 90^\circ C$

$T_{superheated} = T_\circ - T_{dp}$

$= 100 - 90 = 10^\circ C$

2.



Raoult's Law

DoF = 3 − 2 − 1 = 0

(n1, n2, J) (air, H2O)

$y P_{total} = P^*_{H_2O}(T°C)$ → $J P = P^*_{H_2O}(80°C)$

from B.3

$J \times 5260 = 355$

$J = 0.067$ mol H_2O / mol

$1 - J = 0.933$ mol BDA/mol

dry gas balance: $0.9 \times 100 = 0.933\ n_2$

$n_2 = 96.46$ mol

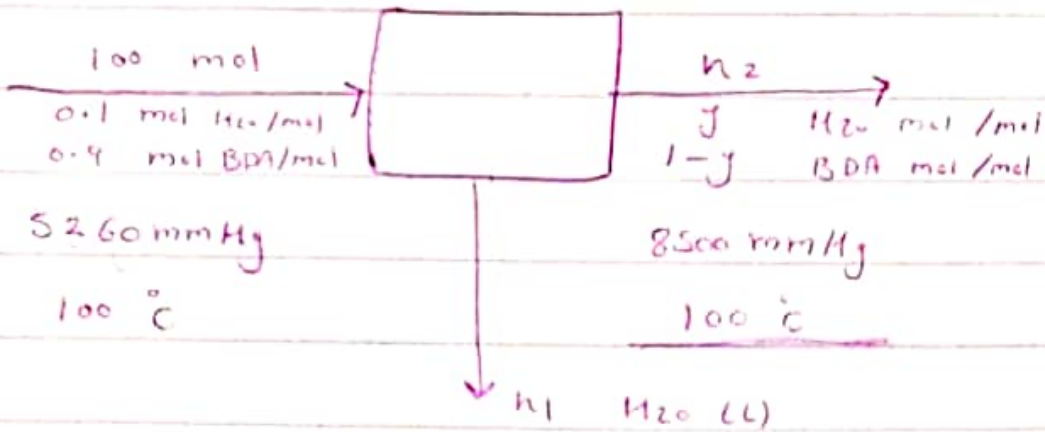
H_2O balance: $0.1 \times 100 = 0.067 \times 100 + n_1$

$n_1 = 3.3$ mol

percentage that condensed = $\frac{3.3 \text{ condensed}}{0.1 \times 100 \text{ feed}} \times 100\%$

= 33 %

3.



$y_{H_2O} P = P^*_{H_2O}(100^\circ C)$ → table B.3

$y \times 8500 = 760$ mmHg $J = 760/8500 = 0.089$ mol H_2O/mol

$1 - J = 0.911$ mol BDA/mol

dry gas balance $0.9 \times 100 = 0.911\, n_2$

$n_2 = 98.7$ mol

H_2O balance $0.1 \times 100 = 0.089 \times 98.7 + n_1$

$n_1 = 1.2157$ mol

Percentage of condensation = $\frac{H_2O \text{ condensed}}{H_2O \text{ feed}} \times 100\%$

$= \frac{1.2157}{0.1 \times 100} \times 100\% = 12\%$

Testyourself p: 254

P^* styrene (82 °C) = 100 mmHg

P^* styrene (100 °C) = 200 mmHg .

Gas : 10% styrene 90% noncondensable

in a tank of 1000 mmHg and 100 °C .

1. dew point ? $y P = P^*(T_{dp})$

$0.1 \times 1000 = P^*(T_{dp})$

$P^*(T_{dp}) = 100$ mmHg

$T_{dp} = 82$ °C

2. relative saturation ?

$$S_r(hr) = \frac{P_i}{P_i^*(T)_{100°C}} \times 100\% = \frac{0.1 \times 1000}{200} = 50\% = 0.5$$

for system

3. molal saturation ? percentage saturation ?

$$S_m(hm) = \frac{P_i}{P - P_i} = \frac{0.1 \times 1000}{1000 - 100} = 1/9$$

$$S_p(\%) = \frac{S_m}{S_m^*} \times 100\% \qquad S_m^* = \frac{P_i^*}{P - P_i^*} = \frac{200}{1000 - 200} = 1/4$$

$$S_P = 1/9 / 1/4 \times 100\% = 44.4\%$$