

Thermo Dynamics 2



**Summer
2025/2026**



Perpared By:

Dr:

Haneen shaltaf

Ali matar

lec 1 :

First law of thermodynamics :

$$(\Delta U + \Delta KE + \Delta PE)_{sys} = \underbrace{Q - W}_{\substack{\text{interaction} \\ \text{surroundings} \rightarrow \text{system} \rightarrow \text{surroundings}}} - \Delta H$$

$\Delta H = 0 \leftarrow$ Closed sys

$Q = 0 \leftarrow$ adiabatic

$Q=0, W=0, \Delta H=0 \leftarrow$ isolated

$W=0 \leftarrow$ No moving parts

- open system → mass, energy, work
- closed system → Energy, work, no mass
- Isolated system → no energy, no work, no mass.

Entropy function behavior :

→ Entropy generation is always positive.

→ At eq in a closed system at constant U and V :

$$S \rightarrow \max, s \rightarrow \max$$

- eq conditions :
- (1) Thermal eq ($T_L = T_V$)
 - (2) Mechanical eq ($P_L = P_V$)
 - (3) Chemical potential ($g_L = g_V$)

EX 7.1-2 : $g = g$ at eq

$$G = H - TS \quad \left(\begin{array}{l} \text{kJ/kg} \\ \text{H, H} \\ \text{S, S} \end{array} \right) \quad \left(\begin{array}{l} \text{kJ/kg} \\ \text{K} \end{array} \right)$$

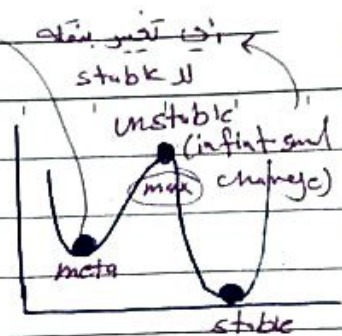
$$* \quad A = U - TS$$

و این حساب ها رو بکنید

در این مثال ها، این دو را مقایسه کنید

(finite change) $\rightarrow$ stable (لا يتغير) $\rightarrow$ stable

$d^2s < 0 \rightarrow$ maximum value of $s \rightarrow$ stable
 $d^2s = 0 \rightarrow$ inflection point of $s \rightarrow$ metastable
 $d^2s > 0 \rightarrow$ minimum value of $s \rightarrow$ unstable



* At eq in a closed system at constant T, V Helmholtz energy must be min.

$A = U - TS = \min$

* At eq in a closed system at constant T and P Gibbs energy must be min.

* At eq in an open system at constant T and P must be min Gibbs energy.

no closed, no dev, also (*)

* Pair of criterion must be satisfied to have stable phase:

① Thermal stability criterion

Heat capacity $\leftarrow C_V = \left(\frac{\partial u}{\partial T} \right)_V > 0 \rightarrow$ internal energy at constant volume must be positive

② Mechanical stability criterion:

Isenthalpic $\leftarrow \kappa_T = -\frac{1}{V} \left(\frac{\partial V}{\partial P} \right)_T > 0 \rightarrow$ compressibility must be positive

lec 2:

molar Gibbs free energy of pure component
↳ Chemical potential (μ)

→ At constant T, P :

* $\mu_{\text{phase 1}} > \mu_{\text{phase 2}} \rightarrow$ species will migrate to the lowest

* $\mu_{\text{Phase 1}} = \mu_{\text{Phase 2}} \rightarrow$ species can exist with equal probability in any of phases.

→ For pure species: chemical potential and molar free energy are synonymous.

→ For mixture → μ is a function of $T, P, \text{composition}$

$$dG = d\mu = -SdT + VdP$$

* μ is a function of $T, P, \text{composition}$

$$\left(\frac{\partial \mu}{\partial T} \right)_P = -S \rightarrow \text{relation between } \mu \text{ and } T \text{ at constant } P$$

فالتالي

* دراسة، للمعادلة

$$\left(\frac{\partial \mu}{\partial P} \right)_T = V \rightarrow \text{relation between } \mu \text{ and } P \text{ at constant } T$$

لو برسم μ مع T

S و V ، μ و T و P متغيرات

$$\Delta \mu = -S \Delta T \rightarrow \text{مقدار}$$

$\Delta \mu$ (J/mol) S (J/K.mol) ΔT (K)

$\Delta \mu$ (J/mol) ΔT (K) S (J/K.mol)

stable, $\Delta \mu < 0$

فإذا $\Delta \mu < 0$ ، $\Delta \mu$ vaporization is spontaneous.

is spontaneous.

$$\Delta \mu = V_m \Delta P \rightarrow P_1$$

$$V_m = \frac{M}{\rho} \rightarrow \text{molar mass (kg/mol)} \quad \text{density } \rho \text{ (kg/m}^3\text{)}$$

$$\Delta \mu = \frac{M \Delta P}{\rho}$$

Phase 1 و Phase 2

Saturated liquid
water at it's triple
point $T = 0.01^\circ\text{C}$

steern 12.1 x
tables

point $T = 0.01^\circ\text{C}$
TD

$$P = 0.6117 \text{ kPa}$$

* در احوال، برکت، در صفا، و برکت

$$T_c = 373.95^\circ\text{C}$$

critical ~~X~~
Point for water

$$P_c = 22.06 \text{ MPa}$$

Equilibrium curve's meaning:

→ Vapor - liquid eq (VLE) → Slope gives the rate of change of the vapor pressure of the liquid with temperature

→ Vapor - Solid → // // // // // // // Vapor
pressure of the solid (Sublimation
with temperature pressure)

liquid - Solid $\rightarrow$ The inverse of the slope, gives the change of melting temperature of the solid with pressure.

* Gauss eqn

$$d_c \left[\frac{dp^{sat}}{dT} \right] = \frac{\Delta S^{sat}}{\Delta V^{sat}}$$

molar vol.

$$\cancel{*} \frac{dS}{dV} = \frac{dH}{T dV} \rightarrow dG$$

الحمد لله الذي جعلنا من آل أبي طالب

* Clapron equation

$$\left[\frac{dp^{\text{sat}}}{dt} = \frac{\Delta H^{\text{sat}}}{T \Delta V^{\text{sat}}} \right] \rightarrow \Delta S^{\text{sat}} = \frac{\Delta H^{\text{sat}}}{T}$$

Clausius Clapeyron equation :

$$\ln\left(\frac{P^{\text{sat}}(T_2)}{P^{\text{sat}}(T_1)}\right) = -\frac{\Delta H^{\text{sat}}}{R} \left(\frac{1}{T_2} - \frac{1}{T_1}\right) \rightarrow \text{Eq. 3}$$

Eq. 3 is valid for liquid and solid

Eq. 3 is valid for liquid and solid

Eq. 3 is valid for liquid and solid

T_1 is the normal boiling point

Eq. 3 is valid for liquid and solid

at the critical point

$$K_p \leftarrow \ln P \approx \frac{1}{T} \rightarrow K$$

$$\frac{-\Delta H}{R} \rightarrow 8.314$$

Estimation of latent Heat of Vaporization

T at Normal boiling point $\rightarrow$ Trouton's rule

T other than normal boiling point $\rightarrow$ Riedel's equation

T other than normal boiling point $\rightarrow$ Watson's correlation

Trouton's rule :

$$\frac{\Delta H}{R T_{\text{NBP}}} = 10$$

ΔH in J/mol, R in J/mol.K, T_{NBP} in K

8.314 J/mol.K

Riedel's equation

$$\frac{\Delta H}{R T} = 1.092 (\ln(P) - 1.013)$$

ΔH in J/mol, R in J/mol.K, T in K, P in bar

$$0.93 - T_{\text{NBP}}$$

$$\frac{T}{T_e}$$

Watson's correlation

$$\frac{\Delta H_e}{\Delta H_i} = \left[\frac{1 - T_2}{1 - T_1} \right]^{0.38}$$

ΔH_e and ΔH_i in J/mol, T_2 and T_1 in K

T_{NBP}

Pitzer's Acentric factor:

$$w = -\log\left(\frac{P_r^{\text{sat}}}{T_r}\right) = 0.7$$

w

- For simple fluids (Ar, Kr, Xe) is zero
- Positive → all other fluids
- Negative → Quantum fluid (H_2 , He, Ne)

lec 3:

→ $G = G^{\text{IG}} + G^{\text{R}}$ Residual Gibbs energy
for ideal gas

→ at eq $G_L^{\text{R}} = G_V^{\text{R}}$

→ Fugacity (هويته) → كلاً كانت عالية
يعني الحالة عند مرتبة بال phase تبعا

$f = p \exp\left[\frac{G^{\text{R}}}{RT}\right] = \phi p$
↓
fugacity coeff
معامل الهويته

$\phi = \exp\left[\frac{G^{\text{R}}}{RT}\right] \rightarrow \ln \phi = \frac{G^{\text{R}}}{RT}$
 $\phi = \frac{f}{p}$

* Chemical equilibrium in terms of fugacity:

$f^{\text{V}} = f^{\text{L}} \leftarrow$ تساوي G^{R} ل Phases بخليتي أحادي
 $\phi^{\text{V}} = \phi^{\text{L}}$
 $G_L^{\text{R}} = G_V^{\text{R}}$ at eq

* تساوي f ل Phases هو دليل شرط كافي للتوازن
ويعطى pure or mixture

* تساوي ϕ ل Phases هو حالة خاصة ل pure

at low p ← mixture لا تتغير مع mixture

* Fugacity in the ideal gas. → ideal gas

$f = p \exp(0) \rightarrow \boxed{f = p}$
 $\phi = \frac{f}{p} = \exp(0) = 1$

الترساق - T-V
phase diagram.

* نقاط خطوط تساوي

نقطة (isobar)

والرقم، المنطقة عليها هي

ال error، لفهم منه قيم ideal gas

Steam tables

* المنطقة الخطية هي

خطاً ضيقاً أقل من 1%

ويستخدم عليها gas ideal

منهج

* الخطاً يزيد مع تزيد

الضغط.

* مجرد ما وصلت، الضغط

الجوي، صار، خطاً كبير

100 KPa

* قيمة، الضغط، خط

منه يتبع، انك من 50

هنا، خط

الضغط، 10 KPa

ويعتبر نقطة، المنطقة

الخطية، ما يتغير مع ideal gas

$G^{\text{R}} = 0 \rightarrow$ مافما
التي بالنسبة ل Ref، G^{IG} هو

* Relationship of Fugacity to the Gibbs energy.

في الحالة المثالية، العلاقة بين $\ln f$ و G هي:

$$\ln \frac{f}{f_0} = \int_{P \rightarrow 0}^P \frac{V}{RT} dP \quad (\text{constant pressure})$$

* في الحالة المثالية، العلاقة بين $\ln f$ و G هي: $G = G^0 + RT \ln f$

في الحالة المثالية، $P \rightarrow 0$

$$\int d(PV) = \int P dV + \int V dP$$

$$\int V dP = PV - \int P dV$$

* Gibbs energy, fugacity and G^0 .

* في الحالة المثالية، العلاقة بين G و f هي:

f

G

* Doesn't require a reference state

* Requires a reference state

(في الحالة المثالية، G^0 هو القيمة المرجعية)

(في الحالة المثالية، G^0 هو القيمة المرجعية)

state

* Has a simple value

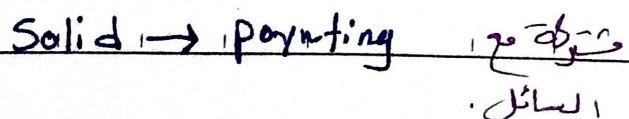
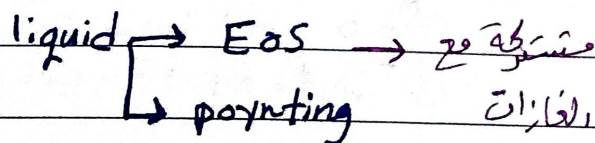
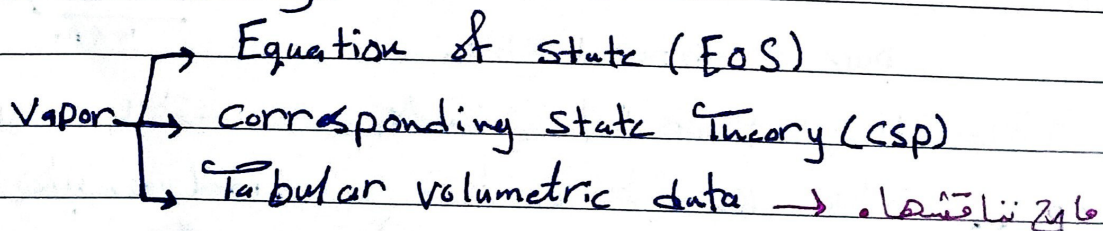
* The value in the ideal

in the ideal gas state gas state ($P \rightarrow 0$).

approaches (∞) $\rightarrow$ في الحالة المثالية، G^0 هو القيمة المرجعية

بالترتيب

* Roadmap to Fugacity:



* Poynting Equation: (liquid / solid)

$$\ln \frac{f}{f_0} = \int_{P_0}^P \frac{v}{RT} dp = \frac{(P - P_0) v}{RT}$$

incompressible liquid, solid

Poynting factor

$$f = f_L \exp \left[\frac{(P - P^{\text{sat}}) v_L}{RT} \right]$$

$$f = \phi^{\text{sat}} p^{\text{sat}} \exp \left[\frac{(P - P^{\text{sat}}) v_L}{RT} \right]$$

saturation

$$P = P^{\text{sat}} \rightarrow f = \phi^{\text{sat}} p^{\text{sat}} \rightarrow \text{Poynting factor}$$

pure comp, ideal gas, liquid

$$\phi^{\text{sat}} = 1$$

$$\phi_v = 1 \text{ ideal gas}$$

$$\text{at eq and pure } \phi_v = \phi_L = 1$$

Ex 7.5 / Ex 7.4

* EOS: (liquid / gas)

ideal gas

$$\ln \phi = Z - 1$$

$$Z = \frac{PV}{RT}$$

Ex 7.7

The virial Eos :

* بتقدير خدد Second virial coeff
منه خلوك معادلة بيتزنر ، أمثا ، الشاتية
والاعمال صحت قد بيدهم

* الرتبة :

لما $B=0$ و الحارة بتكون Boyle's temp وعندها $Z=1$

بس منه ففانه انه ideal gas هو ~~هو~~ هو

لأن $Attractive = Repulsive$ وبالغاز المثالي
احنا بنفرجه إني ما في Molecular force (ملا)

$$(Attractive) \quad Z < 1 \leftarrow B < 0$$

$$(Repulsive) \quad Z > 1 \leftarrow B > 0$$

هذا معناه منه دالتا Z أقل من واحد

* Pitzer's correlations for second virial coeff.

$$Z = 1 + \frac{BP}{RT_c} = 1 + \frac{\hat{B} P_r}{T_r}$$

$$T_r = \frac{T}{T_c}$$

$$T_c = 674.096 K$$

$$P_c = 220.64 \text{ bar}$$

$$\hat{B} = \frac{BP_c}{RT_c} = B^0 + \frac{WB^1}{T_r^{1.6}}$$

$$P_r = \frac{P}{P_c}$$

$$W = 0.344$$

for water

Pitzer

التمحيح

$$B^0 = 0.083 - \frac{0.422}{T_r^{1.6}}$$

* حل المثال

$$B^1 = 0.139 - \frac{0.172}{T_r^{4.2}}$$

$$\ln \phi = Z - 1$$

$$f = \phi P$$

* ولا تنسى

* خطوات حل السؤال :

1) T_r / P_r 2) B^0 3) B^1

4) $\hat{B}$ 5) Z 6) B 7) $V \rightarrow Z = \frac{PV}{RT}$

$$= 1 + \frac{\hat{B} P_r}{T_r}$$

$$Z = 1 + \frac{BP}{RT} \rightarrow P_r$$

$$8.314$$

$$m^3/kg \rightarrow V$$

قسمه الى W

$$= 18 \text{ g/mol} \rightarrow$$

واحدًا بقاءه

بقية ال V بالوجود

Steam

Five Apple

ومائتي ذيل
٧٩

* Generalized compressibility factor

الرسم يوضح z كدالة لـ P_r و T_r

1) Lee-Kesler

2) corresponding state theory

* طريقة بنسب في z مع تلك للرسم

بالم T_r و P_r بنقاط ونطاق z_0

والجيبه بنوع الرسم لشوه z للتمثيل

بعد ما نطرح z_0 و z_1 فان $z = z_0 + w z_1$

* ومعني بنسبنا الطريقة بي ϕ حسب ϕ مع

خلال الى ان $\log \phi = \log \phi^0 + w \log \phi^1$

حسب ϕ و ϕ^0 و ϕ^1 بي ϕ

* و هذا كدالة لفرق بالكمالات z بقدر أصح

z بالم T_r, P_r مع z ان z و بقدر أصح

ϕ بالم T_r, P_r مع ϕ كان ϕ

* حل 7.8 / Ex 7.13

* Van der Waals equation:

$$p = \frac{RT}{V-b} - \frac{a}{V^2}$$

و b حجم الجزيئات (حجم الجزيئات)

No molecular forces

forces

هذا حل مشكلة

الغاز ideal gas

فرض حجم الجزيئات

صفر في ideal gas

+ كانت أول معادلة تنبئه على سائل

وغاز مع بعض

* مشكلة لها مة دقيقة جدًا بالنسبة

للواقع مة دقيقة

Quantitative مة دقيقة

والطاقة بين النقاط مع a بين الأرقام صغير

$$p = \frac{RT}{V}$$

* مة فح على قانون الغاز المثالي

1) low pressure

2) high pressure Temp

* ولكن الافتراضات الجني على قانون

الغاز المثالي:

1) The volume of molecules = 0

2) No Molecular forces between Molecules.

* Fugacity from cubic Equations of state :

* بدنا ضيق 1, fugacity ونا 3 طرق $\rightarrow$ const

1) VdW $\leftarrow$ $A = \frac{ap}{(RT)^2}$ / $B' = \frac{bP}{RT}$ $\leftarrow$ منهم بجزء معادلات معادلة Z

2) SRK

3) PR

من جدول، استلزمات ثم :

$$\ln \phi = \ln \frac{f}{P} = (Z-1) - \ln(Z-B')$$

وحسب ϕ و f

(*) الا حقا لا، والى معادلات تطرح مع

مع المعادلات وينتجها 3 طرق :

1) 3 real roots $\rightarrow$ الأكثر بغيره لا vapor
والأقل لا liquid، لوسط بينهما، وينحسب f
كل حالة منهم وعليه :

والمفرد هو $f^V = f^L$ (Saturation) $\rightarrow$

$f^V < f^L$ (super heated vapor pressure)

$f^L < f^V$ (Subcooled liquid)

$\phi = \frac{f}{P}$ $\rightarrow$ وطبقا بقدر أقاله، ϕ $\rightarrow$ لا، والمفرد نفسه $\phi = \frac{f}{P}$

2) 2 complex, 1 real $\rightarrow$ بقالة قيمة Z بالذات $\rightarrow$ أقرب لـ B (vapor) $\rightarrow$ أقرب لـ A (liquid)

$\rightarrow$ مع نفس البطل بالمعادلات مع قيم لوسط :

1) جذور حقا و P و W للمادة :

2) ضيق B $\rightarrow$ ضيق K $\rightarrow$ $\sqrt{\alpha(T)}$ $\rightarrow$ $\alpha(T)$

4) ضيق A و B

5) نخرج معادلاته $Z^3 + a_2 Z^2 + a_1 Z + a_0 = 0$ حسب جدول المعادلات للطريقة

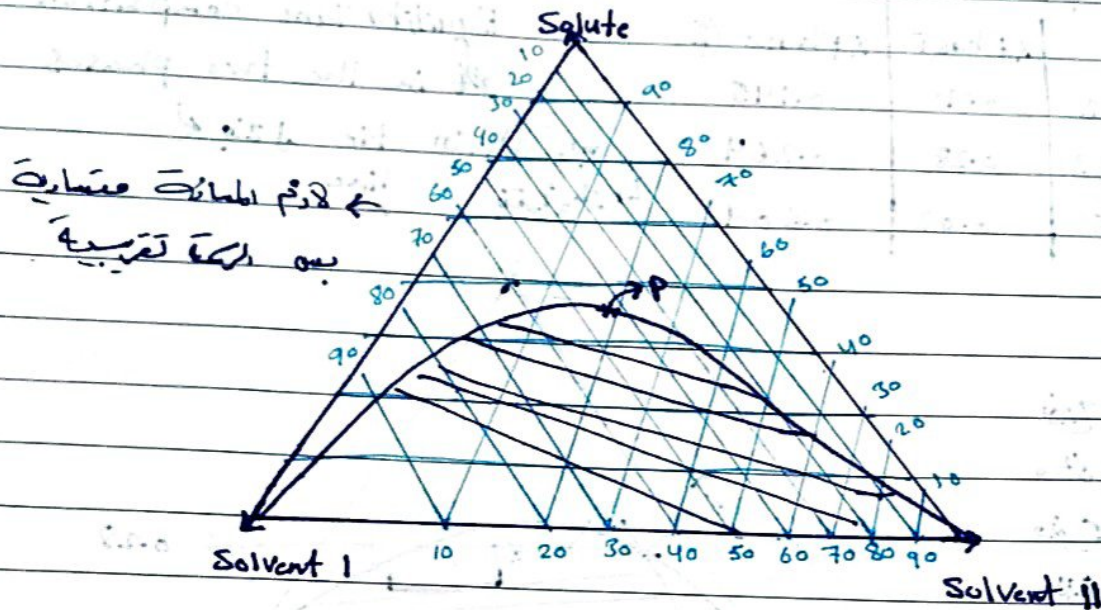
وحسب قيم Z، ونقتطع الجذور الحقا في الأعلى.

6) نستخدم معادلات $\ln \phi$ لكل طريقة معادلتها

ومتقاربه f مع نفسه ال State

* دراسة الرغمة مع استلزمات.

Ternary system :



* P $\rightarrow$ plait point ($K = 1$)

Homogeneous, Heterogeneous

* Positive

solvent 1 $\rightarrow$ tends to solvent ①

الحل :

Ex 8.5

① كتلة Z لكل مادة

$$Z_{\text{water}} = \frac{10}{10 + 10.4 + 10.87} = 0.32$$

$$Z_{\text{aa}} = \frac{10.4}{10 + 10.4 + 10.87} = 0.33$$

$$Z_{\text{mbiv}} = \frac{10.87}{10 + 10.4 + 10.87} = 0.35$$

check $0.35 + 0.33 + 0.32 = 1$ ✓

② ترسيم جدول

* بس رصاي بي

Equilibrium composition
in the two phases

	②	x Phase ①	x Phase ②
water	0.32	0.7	0.145
AA	0.33	0.28	0.264
MIBK	0.35	0.02	0.609

← تيزال النقطة وبه
فترا L_1, L_2 line

③ فوج للرصة

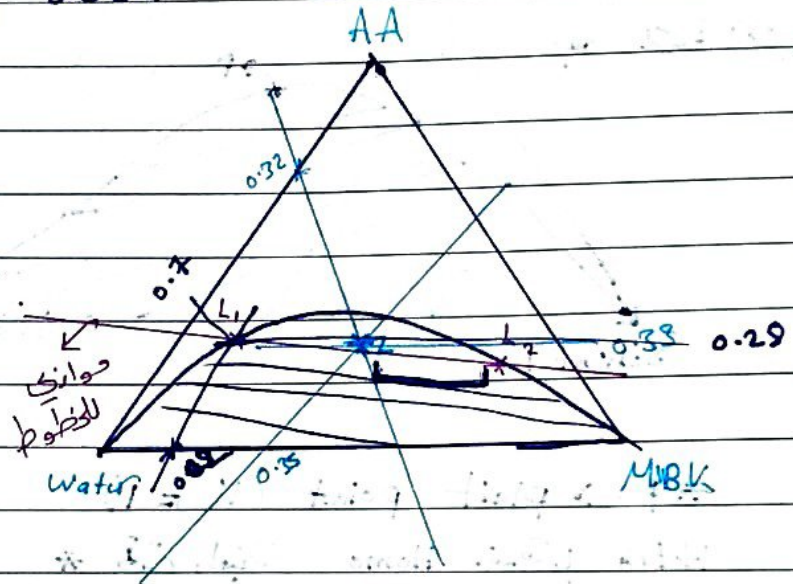
وخذر نقطة Z

ونر كملها tie صوازي

للتقاط L_1 لفتية

وخذر Z و L_1 و L_2

ويفي، كندول



④ calculate :

water $\rightarrow L_1 = \frac{\text{المساحة بين } Z \text{ و } L_2}{Z} = \frac{0.32 - 0.145}{0.7 - 0.145} = 0.32$

(Lever
rule)

AA $\rightarrow L_1 = \frac{0.33 - 0.264}{0.28 - 0.264} =$

MIBK $\rightarrow L_1 = \frac{0.35 - 0.609}{0.02 - 0.609} =$

الرقم
منه منقولة

عشان، التقاط عن نقطة
نقطه مثاليه

water $L_2 = 1 - L_1$

AA $= L_2 = 1 - L_1$

MIBK $= L_2 = 1 - L_1$

to check

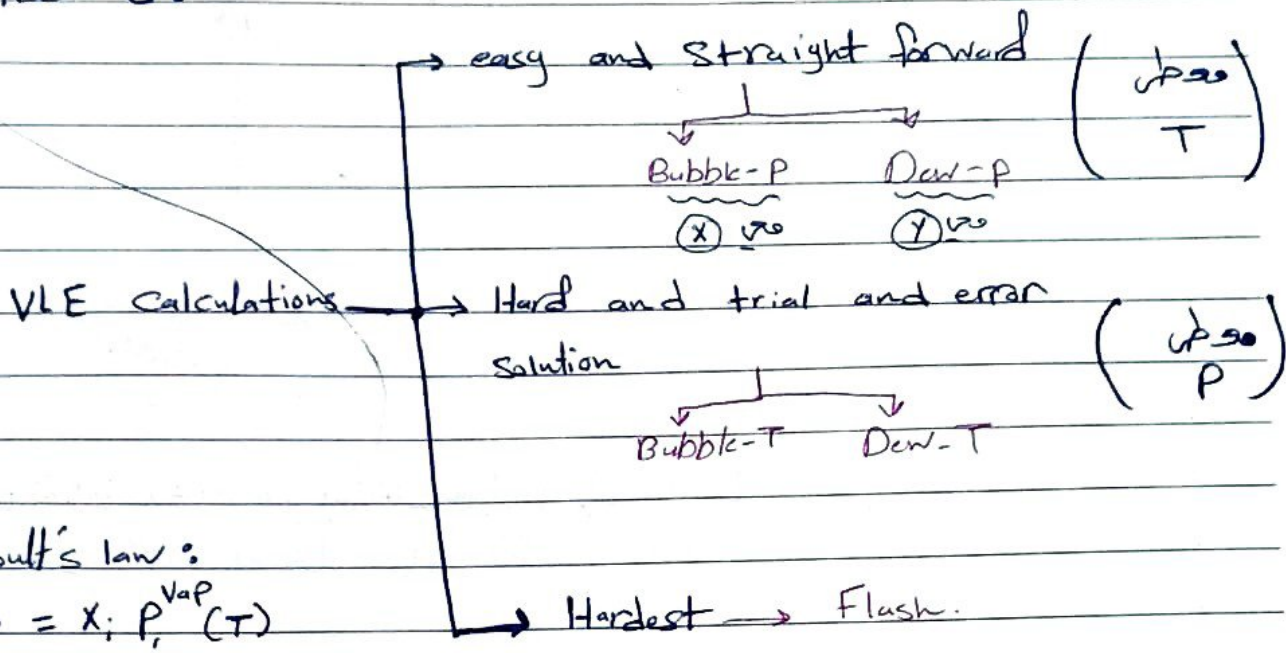
$L_2 = \frac{\text{المساحة بين } L_1 \text{ و } Z}{L_1}$

① K = تركيز
In Phase ①

تركيز
in phase ②

المساحة الكلية

lec 6:



Raoult's law:

$$y_i P = x_i P_i^{vap}(T)$$

متناسب لثابت الجاذبية
متناسب ب

① Size ③ chemical interaction

② shape

في حالة الغازات الحقيقية

ideal gas.

Example (Bubble P)

* يمكن حساب رواتر متجانس و لا ؟ نعم لا

Comp	x_i	A	B	C	P^*	$x_i P^*$	$y_i = \frac{x_i P^*}{P}$
					$= \exp \left[\frac{A-B}{T+C} \right]$ K		
						$P = \text{المجموع}$	① مجموع

* حتى ان كان P^* من P^* الى P^* من P^* الى P^*

* مجموع y يساوي ①

* K_1 على K_2 و K_3 و K_4

في حالة Apply و K_1 و K_2 و K_3 و K_4 و K_5 و K_6 و K_7 و K_8 و K_9 و K_{10} و K_{11} و K_{12} و K_{13} و K_{14} و K_{15} و K_{16} و K_{17} و K_{18} و K_{19} و K_{20} و K_{21} و K_{22} و K_{23} و K_{24} و K_{25} و K_{26} و K_{27} و K_{28} و K_{29} و K_{30} و K_{31} و K_{32} و K_{33} و K_{34} و K_{35} و K_{36} و K_{37} و K_{38} و K_{39} و K_{40} و K_{41} و K_{42} و K_{43} و K_{44} و K_{45} و K_{46} و K_{47} و K_{48} و K_{49} و K_{50} و K_{51} و K_{52} و K_{53} و K_{54} و K_{55} و K_{56} و K_{57} و K_{58} و K_{59} و K_{60} و K_{61} و K_{62} و K_{63} و K_{64} و K_{65} و K_{66} و K_{67} و K_{68} و K_{69} و K_{70} و K_{71} و K_{72} و K_{73} و K_{74} و K_{75} و K_{76} و K_{77} و K_{78} و K_{79} و K_{80} و K_{81} و K_{82} و K_{83} و K_{84} و K_{85} و K_{86} و K_{87} و K_{88} و K_{89} و K_{90} و K_{91} و K_{92} و K_{93} و K_{94} و K_{95} و K_{96} و K_{97} و K_{98} و K_{99} و K_{100} و K_{101} و K_{102} و K_{103} و K_{104} و K_{105} و K_{106} و K_{107} و K_{108} و K_{109} و K_{110} و K_{111} و K_{112} و K_{113} و K_{114} و K_{115} و K_{116} و K_{117} و K_{118} و K_{119} و K_{120} و K_{121} و K_{122} و K_{123} و K_{124} و K_{125} و K_{126} و K_{127} و K_{128} و K_{129} و K_{130} و K_{131} و K_{132} و K_{133} و K_{134} و K_{135} و K_{136} و K_{137} و K_{138} و K_{139} و K_{140} و K_{141} و K_{142} و K_{143} و K_{144} و K_{145} و K_{146} و K_{147} و K_{148} و K_{149} و K_{150} و K_{151} و K_{152} و K_{153} و K_{154} و K_{155} و K_{156} و K_{157} و K_{158} و K_{159} و K_{160} و K_{161} و K_{162} و K_{163} و K_{164} و K_{165} و K_{166} و K_{167} و K_{168} و K_{169} و K_{170} و K_{171} و K_{172} و K_{173} و K_{174} و K_{175} و K_{176} و K_{177} و K_{178} و K_{179} و K_{180} و K_{181} و K_{182} و K_{183} و K_{184} و K_{185} و K_{186} و K_{187} و K_{188} و K_{189} و K_{190} و K_{191} و K_{192} و K_{193} و K_{194} و K_{195} و K_{196} و K_{197} و K_{198} و K_{199} و K_{200} و K_{201} و K_{202} و K_{203} و K_{204} و K_{205} و K_{206} و K_{207} و K_{208} و K_{209} و K_{210} و K_{211} و K_{212} و K_{213} و K_{214} و K_{215} و K_{216} و K_{217} و K_{218} و K_{219} و K_{220} و K_{221} و K_{222} و K_{223} و K_{224} و K_{225} و K_{226} و K_{227} و K_{228} و K_{229} و K_{230} و K_{231} و K_{232} و K_{233} و K_{234} و K_{235} و K_{236} و K_{237} و K_{238} و K_{239} و K_{240} و K_{241} و K_{242} و K_{243} و K_{244} و K_{245} و K_{246} و K_{247} و K_{248} و K_{249} و K_{250} و K_{251} و K_{252} و K_{253} و K_{254} و K_{255} و K_{256} و K_{257} و K_{258} و K_{259} و K_{260} و K_{261} و K_{262} و K_{263} و K_{264} و K_{265} و K_{266} و K_{267} و K_{268} و K_{269} و K_{270} و K_{271} و K_{272} و K_{273} و K_{274} و K_{275} و K_{276} و K_{277} و K_{278} و K_{279} و K_{280} و K_{281} و K_{282} و K_{283} و K_{284} و K_{285} و K_{286} و K_{287} و K_{288} و K_{289} و K_{290} و K_{291} و K_{292} و K_{293} و K_{294} و K_{295} و K_{296} و K_{297} و K_{298} و K_{299} و K_{300} و K_{301} و K_{302} و K_{303} و K_{304} و K_{305} و K_{306} و K_{307} و K_{308} و K_{309} و K_{310} و K_{311} و K_{312} و K_{313} و K_{314} و K_{315} و K_{316} و K_{317} و K_{318} و K_{319} و K_{320} و K_{321} و K_{322} و K_{323} و K_{324} و K_{325} و K_{326} و K_{327} و K_{328} و K_{329} و K_{330} و K_{331} و K_{332} و K_{333} و K_{334} و K_{335} و K_{336} و K_{337} و K_{338} و K_{339} و K_{340} و K_{341} و K_{342} و K_{343} و K_{344} و K_{345} و K_{346} و K_{347} و K_{348} و K_{349} و K_{350} و K_{351} و K_{352} و K_{353} و K_{354} و K_{355} و K_{356} و K_{357} و K_{358} و K_{359} و K_{360} و K_{361} و K_{362} و K_{363} و K_{364} و K_{365} و K_{366} و K_{367} و K_{368} و K_{369} و K_{370} و K_{371} و K_{372} و K_{373} و K_{374} و K_{375} و K_{376} و K_{377} و K_{378} و K_{379} و K_{380} و K_{381} و K_{382} و K_{383} و K_{384} و K_{385} و K_{386} و K_{387} و K_{388} و K_{389} و K_{390} و K_{391} و K_{392} و K_{393} و K_{394} و K_{395} و K_{396} و K_{397} و K_{398} و K_{399} و K_{400} و K_{401} و K_{402} و K_{403} و K_{404} و K_{405} و K_{406} و K_{407} و K_{408} و K_{409} و K_{410} و K_{411} و K_{412} و K_{413} و K_{414} و K_{415} و K_{416} و K_{417} و K_{418} و K_{419} و K_{420} و K_{421} و K_{422} و K_{423} و K_{424} و K_{425} و K_{426} و K_{427} و K_{428} و K_{429} و K_{430} و K_{431} و K_{432} و K_{433} و K_{434} و K_{435} و K_{436} و K_{437} و K_{438} و K_{439} و K_{440} و K_{441} و K_{442} و K_{443} و K_{444} و K_{445} و K_{446} و K_{447} و K_{448} و K_{449} و K_{450} و K_{451} و K_{452} و K_{453} و K_{454} و K_{455} و K_{456} و K_{457} و K_{458} و K_{459} و K_{460} و K_{461} و K_{462} و K_{463} و K_{464} و K_{465} و K_{466} و K_{467} و K_{468} و K_{469} و K_{470} و K_{471} و K_{472} و K_{473} و K_{474} و K_{475} و K_{476} و K_{477} و K_{478} و K_{479} و K_{480} و K_{481} و K_{482} و K_{483} و K_{484} و K_{485} و K_{486} و K_{487} و K_{488} و K_{489} و K_{490} و K_{491} و K_{492} و K_{493} و K_{494} و K_{495} و K_{496} و K_{497} و K_{498} و K_{499} و K_{500} و K_{501} و K_{502} و K_{503} و K_{504} و K_{505} و K_{506} و K_{507} و K_{508} و K_{509} و K_{510} و K_{511} و K_{512} و K_{513} و K_{514} و K_{515} و K_{516} و K_{517} و K_{518} و K_{519} و K_{520} و K_{521} و K_{522} و K_{523} و K_{524} و K_{525} و K_{526} و K_{527} و K_{528} و K_{529} و K_{530} و K_{531} و K_{532} و K_{533} و K_{534} و K_{535} و K_{536} و K_{537} و K_{538} و K_{539} و K_{540} و K_{541} و K_{542} و K_{543} و K_{544} و K_{545} و K_{546} و K_{547} و K_{548} و K_{549} و K_{550} و K_{551} و K_{552} و K_{553} و K_{554} و K_{555} و K_{556} و K_{557} و K_{558} و K_{559} و K_{560} و K_{561} و K_{562} و K_{563} و K_{564} و K_{565} و K_{566} و K_{567} و K_{568} و K_{569} و K_{570} و K_{571} و K_{572} و K_{573} و K_{574} و K_{575} و K_{576} و K_{577} و K_{578} و K_{579} و K_{580} و K_{581} و K_{582} و K_{583} و K_{584} و K_{585} و K_{586} و K_{587} و K_{588} و K_{589} و K_{590} و K_{591} و K_{592} و K_{593} و K_{594} و K_{595} و K_{596} و K_{597} و K_{598} و K_{599} و K_{600} و K_{601} و K_{602} و K_{603} و K_{604} و K_{605} و K_{606} و K_{607} و K_{608} و K_{609} و K_{610} و K_{611} و K_{612} و K_{613} و K_{614} و K_{615} و K_{616} و K_{617} و K_{618} و K_{619} و K_{620} و K_{621} و K_{622} و K_{623} و K_{624} و K_{625} و K_{626} و K_{627} و K_{628} و K_{629} و K_{630} و K_{631} و K_{632} و K_{633} و K_{634} و K_{635} و K_{636} و K_{637} و K_{638} و K_{639} و K_{640} و K_{641} و K_{642} و K_{643} و K_{644} و K_{645} و K_{646} و K_{647} و K_{648} و K_{649} و K_{650} و K_{651} و K_{652} و K_{653} و K_{654} و K_{655} و K_{656} و K_{657} و K_{658} و K_{659} و K_{660} و K_{661} و K_{662} و K_{663} و K_{664} و K_{665} و K_{666} و K_{667} و K_{668} و K_{669} و K_{670} و K_{671} و K_{672} و K_{673} و K_{674} و K_{675} و K_{676} و K_{677} و K_{678} و K_{679} و K_{680} و K_{681} و K_{682} و K_{683} و K_{684} و K_{685} و K_{686} و K_{687} و K_{688} و K_{689} و K_{690} و K_{691} و K_{692} و K_{693} و K_{694} و K_{695} و K_{696} و K_{697} و K_{698} و K_{699} و K_{700} و K_{701} و K_{702} و K_{703} و K_{704} و K_{705} و K_{706} و K_{707} و K_{708} و K_{709} و K_{710} و K_{711} و K_{712} و K_{713} و K_{714} و K_{715} و K_{716} و K_{717} و K_{718} و K_{719} و K_{720} و K_{721} و K_{722} و K_{723} و K_{724} و K_{725} و K_{726} و K_{727} و K_{728} و K_{729} و K_{730} و K_{731} و K_{732} و K_{733} و K_{734} و K_{735} و K_{736} و K_{737} و K_{738} و K_{739} و K_{740} و K_{741} و K_{742} و K_{743} و K_{744} و K_{745} و K_{746} و K_{747} و K_{748} و K_{749} و K_{750} و K_{751} و K_{752} و K_{753} و K_{754} و K_{755} و K_{756} و K_{757} و K_{758} و K_{759} و K_{760} و K_{761} و K_{762} و K_{763} و K_{764} و K_{765} و K_{766} و K_{767} و K_{768} و K_{769} و K_{770} و K_{771} و K_{772} و K_{773} و K_{774} و K_{775} و K_{776} و K_{777} و K_{778} و K_{779} و K_{780} و K_{781} و K_{782} و K_{783} و K_{784} و K_{785} و K_{786} و K_{787} و K_{788} و K_{789} و K_{790} و K_{791} و K_{792} و K_{793} و K_{794} و K_{795} و K_{796} و K_{797} و K_{798} و K_{799} و K_{800} و K_{801} و K_{802} و K_{803} و K_{804} و K_{805} و K_{806} و K_{807} و K_{808} و K_{809} و K_{810} و K_{811} و K_{812} و K_{813} و K_{814} و K_{815} و K_{816} و K_{817} و K_{818} و K_{819} و K_{820} و K_{821} و K_{822} و K_{823} و K_{824} و K_{825} و K_{826} و K_{827} و K_{828} و K_{829} و K_{830} و K_{831} و K_{832} و K_{833} و K_{834} و K_{835} و K_{836} و K_{837} و K_{838} و K_{839} و K_{840} و K_{841} و K_{842} و K_{843} و K_{844} و K_{845} و K_{846} و K_{847} و K_{848} و K_{849} و K_{850} و K_{851} و K_{852} و K_{853} و K_{854} و K_{855} و K_{856} و K_{857} و K_{858} و K_{859} و K_{860} و K_{861} و K_{862} و K_{863} و K_{864} و K_{865} و K_{866} و K_{867} و K_{868} و K_{869} و K_{870} و K_{871} و K_{872} و K_{873} و K_{874} و K_{875} و K_{876} و K_{877} و K_{878} و K_{879} و K_{880} و K_{881} و K_{882} و K_{883} و K_{884} و K_{885} و K_{886} و K_{887} و K_{888} و K_{889} و K_{890} و K_{891} و K_{892} و K_{893} و K_{894} و K_{895} و K_{896} و K_{897} و K_{898} و K_{899} و K_{900} و K_{901} و K_{902} و K_{903} و K_{904} و K_{905} و K_{906} و K_{907} و K_{908} و K_{909} و K_{910} و K_{911} و K_{912} و K_{913} و K_{914} و K_{915} و K_{916} و K_{917} و K_{918} و K_{919} و K_{920} و K_{921} و K_{922} و K_{923} و K_{924} و K_{925} و K_{926} و K_{927} و K_{928} و K_{929} و K_{930} و K_{931} و K_{932} و K_{933} و K_{934} و K_{935} و K_{936} و K_{937} و K_{938} و K_{939} و K_{940} و K_{941} و K_{942} و K_{943} و K_{944} و K_{945} و K_{946} و K_{947} و K_{948} و K_{949} و K_{950} و K_{951} و K_{952} و K_{953} و K_{954} و K_{955} و K_{956} و K_{957} و K_{958} و K_{959} و K_{960} و K_{961} و K_{962} و K_{963} و K_{964} و K_{965} و K_{966} و K_{967} و K_{968} و K_{969} و K_{970} و K_{971} و K_{972} و K_{973} و K_{974} و K_{975} و K_{976} و K_{977} و K_{978} و K_{979} و K_{980} و K_{981} و K_{982} و K_{983} و K_{984} و K_{985} و K_{986} و K_{987} و K_{988} و K_{989} و K_{990} و K_{991} و K_{992} و K_{993} و K_{994} و K_{995} و K_{996} و K_{997} و K_{998} و K_{999} و K_{1000}

$$K = \frac{y}{x}$$

$$\alpha_{12} = \frac{K_1}{K_2}$$

$$\alpha_{13} = \frac{K_1}{K_3}$$

$$\alpha_{23} = \frac{K_2}{K_3}$$

$$0.95 < \alpha < 1.05$$

* بقدر اقرب سهل
كبره سهل
لـ α افضل او 8

① يساوي
* K_1 على K_2 و K_3 و K_4
* K_1 و K_2 و K_3

Example (Dew - P)

Component

γ_i

A

B

C

P^*

مثال جديد

$$\frac{\gamma_i}{P_i^*}$$

$$x_i = \left(\frac{\gamma_i}{P_i^*} \right) * P$$

$P =$

مقابل المجموع

ما تفوت عن شان هي بس نقدر على الكرامة، الكرامة نفسها
باقا، شروط كلها نفسها، شان نتأكد لو صح.

lec 7:

T like log P like *

Bubble - T:

$$① T = \frac{B}{A - \ln^{v.p} P} - C \rightarrow \text{قائمة بنوعها}$$

$$P = P^{v.p}$$

$$② T = \sum X_i T_i \rightarrow T \rightarrow \text{initial guess}$$

component	X_i	A	B	C	P^*	$X_i P_i^*$	$Y_i = \frac{X_i P_i^*}{P}$
							الـ P بالسؤال
							منه واحد

$P = \text{المجموع}$

ملاحظة مع P بالسؤال

(ناتج Y)

مقبول كد واحد باللمة

ما طرح قريب من الواحد كد واحد باللمة ؟

مع قنار اول مادة مفتاحية ونقسم P^* تبعها على مجموع Y ونستخدم مرجع ونرجع طب T (Key comp)

$$T = \frac{B}{A - \ln^{v.p} P} - C \quad \left(\begin{array}{l} \text{كل الاشياء للمادة} \\ \text{المفتاحية} \end{array} \right)$$

→ T ما معي جديدة

كل جدول مني عليها

$$\exp\left[A - \frac{B}{T+C}\right]$$

comp	X_i	A	B	C	P^*	$X_i P^*$	$Y = \frac{X_i P^*}{P}$
							الـ P بالسؤال

اعداد صواب

كل اعداد جديدة

وهذا حتى $1 - \epsilon y$

< 0.0001

Ans - T :

① $T = \frac{B}{A - \ln p} \rightarrow \bar{p}, \bar{b}, \bar{y}, \bar{v}$

(2) $T = \sum y T$ (افزایش)

[illegible]

المجموع، مقارنة
بخط أسود

تجميع الـ X

لازم تعدادی واحد خود فرجه ۱ باشد

8 8 2

ج. (نقص) P^* لا Key بال x ونرج حسب T ونرج كل

$$PB = \sum x p^*$$

$$PD = \frac{1}{\sum \frac{g}{p^*}}$$

Ex: $T = 323.15 \text{ K}$
 $P = 1025 \text{ KPa}$

we have

$\left(\frac{P^*}{P}\right)$

comp	z	P^* (KPa)	K_i	$K_i - 1$
propane	0.5	1681.4	1.6404	0.6404
i-butane	0.25	674.2	0.6578	-0.3422
n-butane	0.25	492.63	0.4806	-0.5194
$z(K_i - 1)$	$\frac{z_i(K_i - 1)}{1 + V(K_i - 1)}$		$X_i = \frac{z_i}{1 + V(K_i - 1)}$	$Y_i = \frac{z_i K_i}{1 + V(K_i - 1)}$
0.3202	0.2588		0.4041	0.6629
-0.08553	-0.09797		0.2863	0.1883
-0.1299	-0.1609		0.3096	0.1484
Sum	0.00008		1	1.0001

(FF) eq:

$$\frac{z_1(K_1 - 1)}{1 + V(K_1 - 1)} + \frac{z_2(K_2 - 1)}{1 + V(K_2 - 1)} + \frac{z_3(K_3 - 1)}{1 + V(K_3 - 1)}$$

by derivation

$$\alpha V^2 + \beta V + \gamma = 0 \quad \leftarrow \quad 0.1138 V^2 - 0.325 V + 0.1048 = 0$$

$$\alpha = (K_1 - 1)(K_2 - 1)(K_3 - 1) = 0.1138$$

$$\beta = (K_1 - 1)(K_2 - 1)(z_1 + z_2) + (K_1 - 1)(K_3 - 1)(z_1 + z_3) + (K_2 - 1)(K_3 - 1)(z_2 + z_3)$$

$$= -0.3250$$

$$\gamma = z_1(K_1 - 1) + z_2(K_2 - 1) + z_3(K_3 - 1) = 0.1048$$

$V = 0.3705$
 $V \neq 2.4853$
 $0 < V < 1$

10 check

- ① z between x and y ✓
- ② The sum of x and y should be 1 ✓
(slight difference due to rounding)
- ③ we have $K > 1$ and $K < 1$ ✓
- ④ Sum of $\frac{z_i(K_i - 1)}{K_i V(K_i - 1)}$ should be zero ✓
(slight difference due to rounding)
- ⑤ $0 < V < 1$ ✓

$$P_B = \sum z P^* = 1132.4075 \text{ kPa}$$

$$P_D = \frac{1}{\sum \frac{z}{P^*}} = 850.5851 \text{ kPa}$$

- ⑥ $P_D < P < P_B \rightarrow 850.5851 < 1025 < 1132.4075$ ✓
can be flashing (mixture).

$$\alpha_{12} = \frac{K_1}{K_2} = 2.4939$$

$$\alpha_{13} = \frac{K_1}{K_3} = 3.4110$$

$$\alpha_{23} = \frac{K_2}{K_3} = 1.3686$$

Alpha is not
 $0.95 \leq \alpha \leq 1.05$

yes we can use
distillation to separate.
but it won't be
very easy because it's
close

$$RT \ln \gamma_i = g^{ex} = \left(\frac{\partial N g^{ex}}{\partial N_i} \right)_{T, P, N_2}$$

$$\frac{g^{ex}}{RT} = A x_1 x_2$$

$$RT \ln \gamma_i = \left(\frac{\partial N A x_1 x_2 RT}{\partial N_i} \right)_{T, P, N_2}$$

$$RT \ln \gamma_i = A RT \left(\frac{\partial N x_1 x_2}{\partial N_i} \right)_{T, P, N_2}$$

$$\ln \gamma_i = A \left(\frac{\partial N \left(\frac{N_1}{N} \right) \left(\frac{N_2}{N} \right)}{\partial N_i} \right)_{T, P, N_2}$$

$$x_1 = \frac{N_1}{N_1 + N_2}$$

$$x_2 = \frac{N_2}{N_1 + N_2}$$

$$N = N_1 + N_2$$

$$\ln \gamma_1 = A \left(\frac{\partial N_1 N_2 / (N_1 + N_2)}{\partial N_1} \right)_{T, P, N_2}$$

$$= A \left(\frac{(N_1 + N_2) N_2 - N_1 N_2}{(N_1 + N_2)^2} \right) = A \left(\frac{N_1 N_2 + N_2^2 - N_1 N_2}{(N_1 + N_2)^2} \right)$$

$$= A \left(\frac{N_2^2}{(N_1 + N_2)^2} \right) = \boxed{A x_2^2}$$

$$\ln \gamma_2 = A \left(\frac{\partial N_1 N_2 / (N_1 + N_2)}{\partial N_2} \right)_{T, P, N_1} = A \left(\frac{(N_1 + N_2) N_1 - N_1 N_2}{(N_1 + N_2)^2} \right)$$

$$= A \left(\frac{N_1^2}{(N_1 + N_2)^2} \right) = \boxed{A x_1^2}$$

(G-D)

$$x_1 \left(\frac{\partial \ln \gamma_1}{\partial x_1} \right) + x_2 \left(\frac{\partial \ln \gamma_2}{\partial x_1} \right) \stackrel{?}{=} 0$$

$$A x_1 \left(\frac{\partial x_2^2}{\partial x_1} \right) + A x_2 \left(\frac{\partial x_1^2}{\partial x_1} \right) \stackrel{?}{=} 0$$

$$A x_1 \left(\frac{\partial (1-x_1)^2}{\partial x_1} \right) = 2(1-x_1) \times -1 = -2A x_1 x_2$$

$$A x_2 \left(\frac{\partial x_1^2}{\partial x_1} \right) = \boxed{2A x_1 x_2}$$

$$-2A x_1 x_2 + 2A x_1 x_2 = 0$$

Consistent

$$\ln \gamma_1 = A x_2^2$$

$$\ln \gamma_2 = A x_1^2$$

$$x_1 \left(\frac{\partial \ln \gamma_1}{\partial x_1} \right) + x_2 \left(\frac{\partial \ln \gamma_2}{\partial x_1} \right) \stackrel{?}{=} 0$$

$$A x_1 \left(\frac{\partial x_1^2}{\partial x_1} \right) = \boxed{2 A x_1^2}$$

$$A x_2 \left(\frac{\partial x_2^2}{\partial x_1} \right) = A x_2 \left(\frac{\partial (1 - x_1^2)}{\partial x_1} \right) = A x_2^2 - 2(1 - x_1) = \boxed{-2 A x_2^2}$$

$$2 A x_1^2 - 2 A x_2^2 \neq 0$$

Not consistent

$$\ln \gamma_1 = A x_2^2$$

$$\ominus \ln \gamma_2 = A x_1^2$$

$$\ln \left(\frac{\gamma_1}{\gamma_2} \right) = A x_2^2 - A x_1^2$$

$$\gamma_1 = \frac{\gamma_1^* P}{x_1 P^*} = \frac{P}{P_1^*}$$

$$\gamma_2 = \frac{P}{P_2^*}$$

$$\frac{\gamma_1}{\gamma_2} = \frac{P_2^*}{P_1^*} = \text{O}$$

$$\leftarrow \textcircled{\gamma_1} = \frac{\gamma_1^* P}{x_1 P^*}$$

$$\ln \gamma_1 = A x_2^2$$

$$\textcircled{\gamma_1}$$

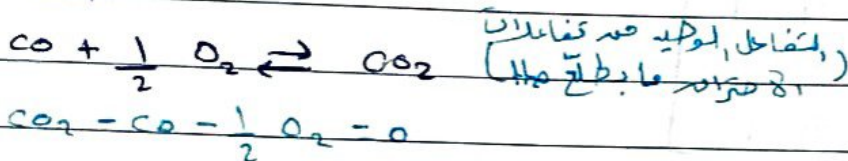
lec 10:

Notation of Chemical Reactions.

* $\sum$ ج كوك، المعادلة من سهم $\rightarrow$
المعادلات بنسب سالبة، المتوازي مع

v for inert = 0

Ex 1:



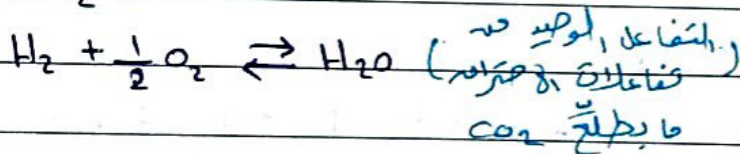
$$CO_2 - CO - \frac{1}{2} O_2 = 0$$

$$v_{CO_2} = 1$$

$$v_{CO} = -1$$

$$v_{O_2} = -\frac{1}{2}$$

Ex 2:



$$H_2O - H_2 - \frac{1}{2} O_2 = 0$$

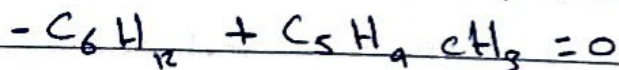
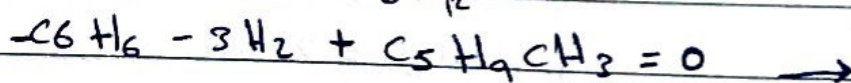
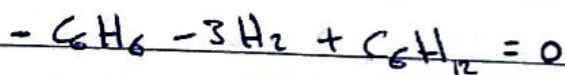
$$v_{H_2O} = 1$$

$$v_{H_2} = -1$$

$$v_{O_2} = -\frac{1}{2}$$

* لا كثر من معادلة بل نفس المعادلة
matrix

Ex:



C_6H_6	H_2	C_6H_{12}	$C_5H_9CH_3$	
-1	-3	1	0	Row 1
-1	-3	0	1	Row 2
0	0	-1	1	Row 3

هذا النظام من المعادلات خطية أم لا؟
 The rank of the matrix.
 (independent) المعادلات المستقلة = dependent

How?

مثال:

Pivot السطر المحتوي على العدد الأكبر	←	2	5	4	1
←	3	6	0	2	
←	4	7	8	1	

العدد الأكبر في السطر

لا توجد أصفار

No zeros in rows → All reaction are independent
 and The rank = Number of rows

Molar extent of reaction:

→ $\xi = n_j - n_{j,0}$ عدد التفاعل

→ at $t = 0$ $\xi = 0$

السرعة
 v_j
 stoich.

* conversion $X = \frac{n_{j,0} - n_j}{n_{j,0}}$

$n_j = \xi v_j + n_{j,0}$
 mole numbers.

limiting reagent

* mole fraction from extent of reaction

$y_j = \frac{n_{j,0} + v_j \xi}{\sum n_{j,0} + \sum v_j \xi}$

Ex:



$n_{j,0}(\text{CH}_4) = 2 \text{ mol}$

$n_{j,0}(\text{H}_2\text{O}) = 1 \text{ mol}$

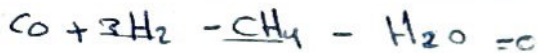
$n_{j,0}(\text{CO}) = 1 \text{ mol}$

$n_{j,0}(\text{H}_2) = 4 \text{ mol}$

① كتلة المواد المتفاعلة

بعد التحويل من حجم

ليساوي



② $\sum V = 1 + 3 - 1 - 1 = 2$

③ $\sum n_{j,0} = 2 + 1 + 1 + 4 = 8$

④ $\bar{P}$ لا يتغير، $\bar{V}$ يتغير

$$y_j = \frac{n_{j,0} + v_j \xi}{\sum n_{j,0} + \sum v_j \xi}$$

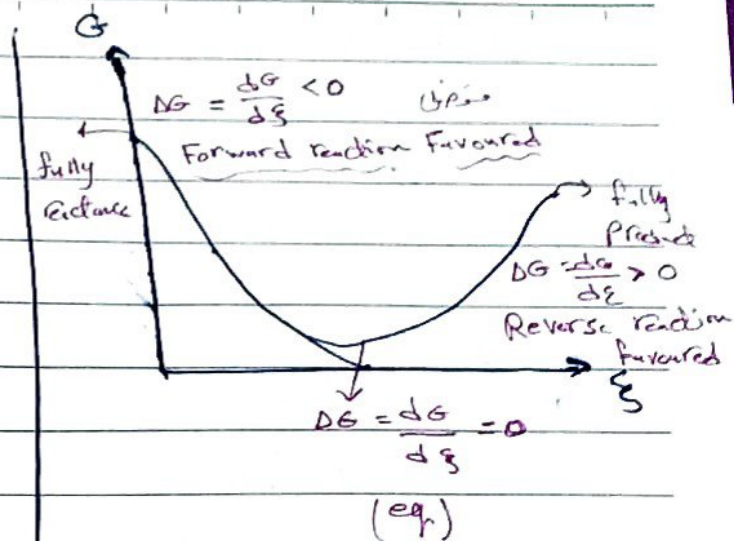
$$y_{\text{CH}_4} = \frac{2 - \xi}{8 + 2\xi}$$

$$y_{\text{CO}} = \frac{1 + \xi}{8 + 2\xi}$$

$$y_{\text{H}_2\text{O}} = \frac{1 - \xi}{8 + 2\xi}$$

$$y_{\text{H}_2} = \frac{4 + 3\xi}{8 + 2\xi}$$

$$y_{\text{CO}} = \frac{1 + \xi}{8 + 2\xi}$$



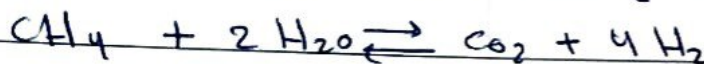
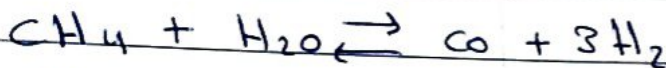
Extent of reaction, for multiple reactions:

$$n_j = n_{j,0} + \sum_i \sum_v \nu_{ij} \xi_i$$

$$y_j = \frac{n_{j,0} + \sum_{i=1}^R \nu_{ij} \xi_i}{\sum n_0 + \sum_i \nu_i \xi_i}$$

$$\sum n_0 + \sum_i \nu_i \xi_i$$

EX:



$$n_0(\text{CH}_4) = 2$$

$$\text{H}_2\text{O} = 3$$

→ initial moles

$$\textcircled{1} -\text{CH}_4 - \text{H}_2\text{O} + \text{CO} + 3\text{H}_2 = 0$$

$$\textcircled{2} \text{CO}_2 + 4\text{H}_2 - \text{CH}_4 - 2\text{H}_2\text{O} = 0$$

CH ₄	H ₂ O	CO	CO ₂	H ₂	ν_i
-1	-1	1	0	3	2
-1	-2	0	1	4	2

→ stoichiometric coefficients

$$\textcircled{3} \sum n_0 = 2 + 3 = 5$$

④ variables

$$y_{\text{CO}} = \frac{\xi_1}{5 + 2\xi_1 + 2\xi_2}$$

$$y_j = \frac{n_{j,0} + \nu_{j1}\xi_1 + \nu_{j2}\xi_2}{\sum n_0 + \sum \nu_{j1}\xi_1 + \sum \nu_{j2}\xi_2}$$

$$y_{\text{CO}_2} = \frac{\xi_2}{5 + 2\xi_1 + 2\xi_2}$$

$$y_{\text{CH}_4} = \frac{2 - \xi_1 - \xi_2}{5 + 2\xi_1 + 2\xi_2}$$

$$y_{\text{H}_2} = \frac{3\xi_1 + 4\xi_2}{5 + 2\xi_1 + 2\xi_2}$$

$$y_{\text{H}_2\text{O}} = \frac{3 - \xi_1 - 2\xi_2}{5 + 2\xi_1 + 2\xi_2}$$