Chapter 6 – 1) restoring composition as a variable.
2) free energy minimization.

Lecture 10.1 2021

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c → components → the c conservative extensive properties of a system
→ isolated system $c = \{U, V, N_1 \dots N_k\}$, $c = k+2$
→ thermodynamic components
→ chemical components k → the min number of chemical entities necessary to describe all possible compositions of a system, $k \geq 1$, $c > k$ (problems 2.1, 4.3), $c < k$

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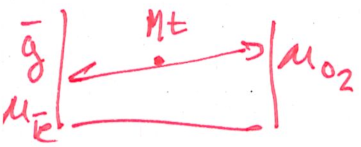
specific g → g^m - molar gibbs → G/mole of phase
→ no chemistry
$\alpha = 1$ mole of phase ; ~~unlike~~ gases, a mole of solid is arbitrary SiO_2; S_2O_4; etc
→ chemistry
→ $\bar{g}$ – gibbs energy per mole of a systems components → defined only in the context of a system. $\alpha = \sum^{k} N_i$



$$\Rightarrow G(P, T, N_{Fe}, N_{O_2}) = \mu_{Fe} N_{Fe} + \mu_{O_2} N_{O_2}$$

$$\bar{g} = G/(N_{Fe} + N_{O_2}) = \mu_{Fe}\bar{n}_{Fe} + \mu_{O_2}\bar{n}_{O_2}$$

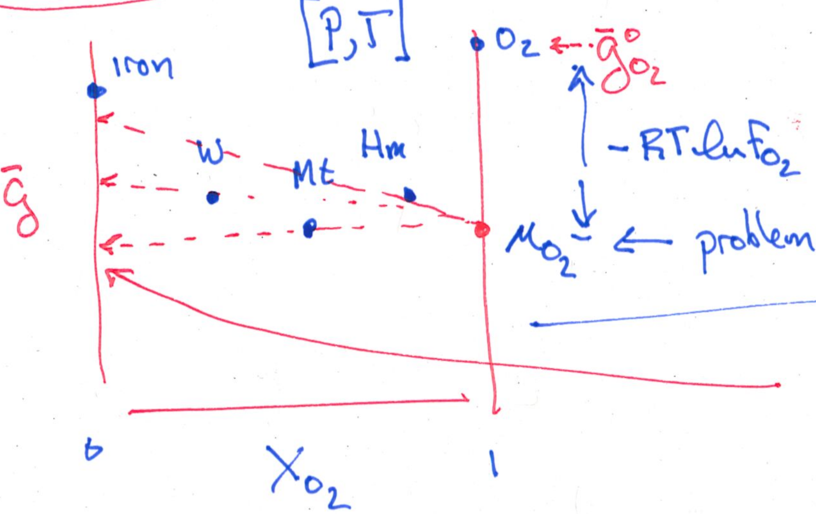
$$\Rightarrow \sum \bar{n} = 1, \quad \bar{n} \to X \quad \Rightarrow \bar{g} = \mu_{Fe}X_{Fe} + \mu_{O_2}X_{O_2}$$

$$\bar{g} = \mu_{Fe}(1 - X_{O_2}) + \mu_{O_2}X_{O_2}$$

$$\bar{g} = \mu_{Fe} + X_{O_2}(\mu_{O_2} - \mu_{Fe})$$

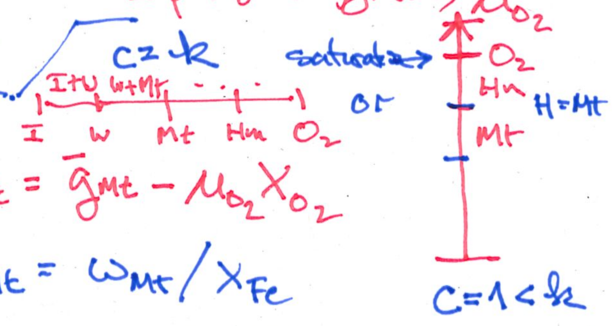
$$\underline{\bar{G} = G^m / \sum n^m}$$

[P, T]



← problem 4.2

2 phase diagrams



$$\omega_{Mt} = \bar{g}_{Mt} - \mu_{O_2}X_{O_2}$$

$$\bar{\omega}_{Mt} = \omega_{Mt} / X_{Fe}$$

Linear programming → Industrial Engineering / operations research

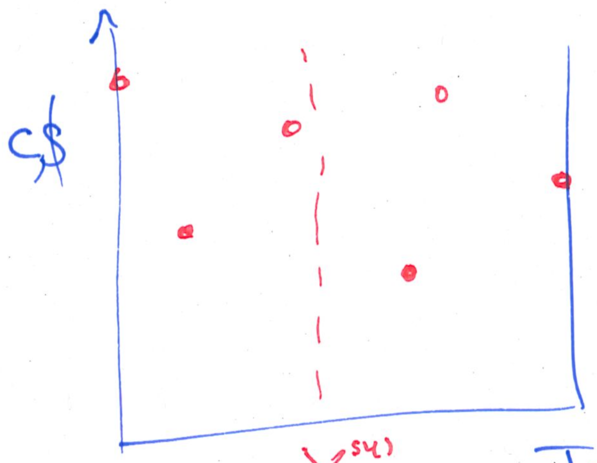
Lecture 10.3 2021

→ resource allocation problems

→ truck manufacture allocate scarce resources

e.g. people + iron

→ factories operate at fixed cost per truck, c^j, with specific resource allocation determined by technology.



1) Π factories, off $\alpha = 0$, on $\alpha > 0$

2) the ratio of available resources determines $X^{sys}_{iron} = 1 - X^{sys}_{people}$

3) minimize total cost (objective function) $C^{TOTAL} = \sum^{\Pi} \alpha^j C^j$

4) subject to constraints:

Linear equalities → $n_{equalities}$

$$X^{system}_{iron} = \sum^{\Pi} \alpha^j X^j_{iron}$$

$$X^{system}_{people} = \sum^{\Pi} \alpha^j X^j_{people}$$

~~Linear~~ Inequalities (Π)

$$\alpha^j \geq 0 \quad j = 1 \ldots \Pi$$

5) the solution will always yield $n = n_{equalities}$ factories with $\alpha^j > 0$

$$G^{sys} = \sum^{\Pi} \alpha^j G^j$$

c - linear equalities

$$X^{sys}_c = \sum_j^{\Pi} \alpha^j X^j_c \quad c = 1 \ldots c$$

inequalities

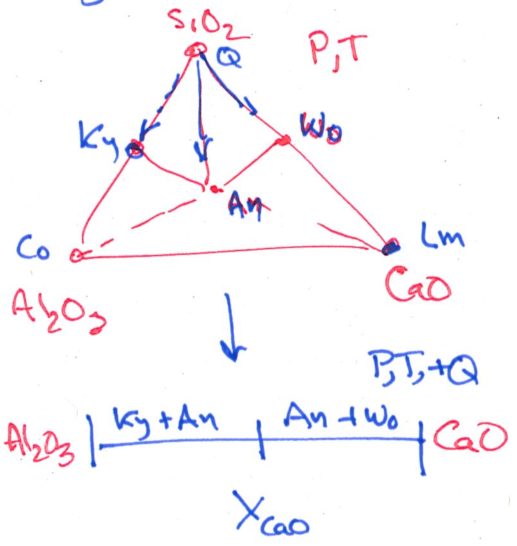
$\alpha^j \geq 0 \Rightarrow$ yield $p = c$ phases w $\alpha^j > 0$

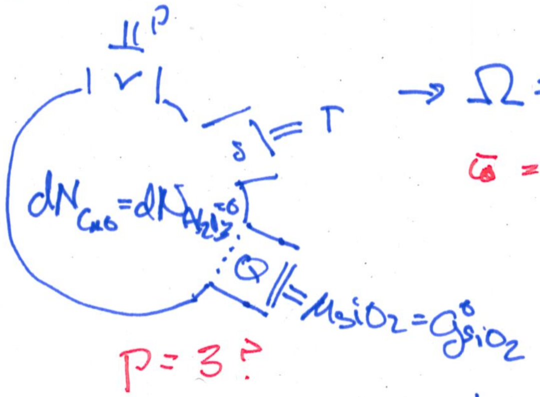
→ if the LHS is extensive then the amounts α^j are absolute

→ if the LHS is specific then the amounts α^j are relative ($\sum \alpha^j = 1$)

lecture 10.2 2021

Petrologic projections = Legendre Transform

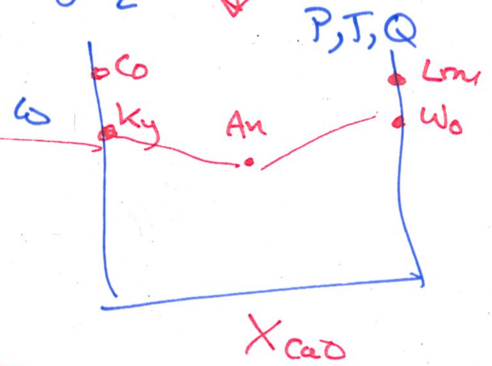




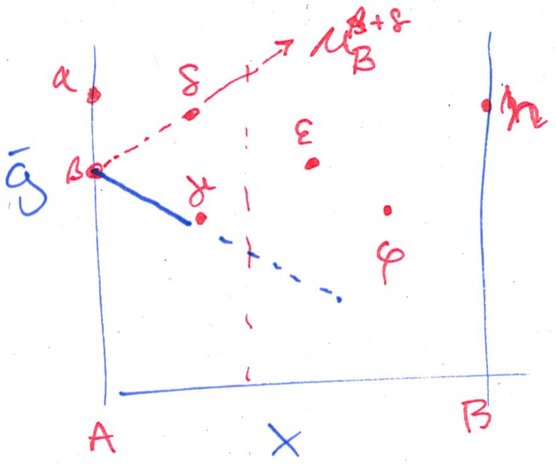
P = 3 ?
P = 2

$\to \Omega = G - N_{SiO_2}\mu_{SiO_2}$

$\bar{\Omega} = \mu_{Al_2O_3}X_{Al_2O_3} + \mu_{CaO}X_{CaO}$



Free energy minimization → phases w/ fixed composition



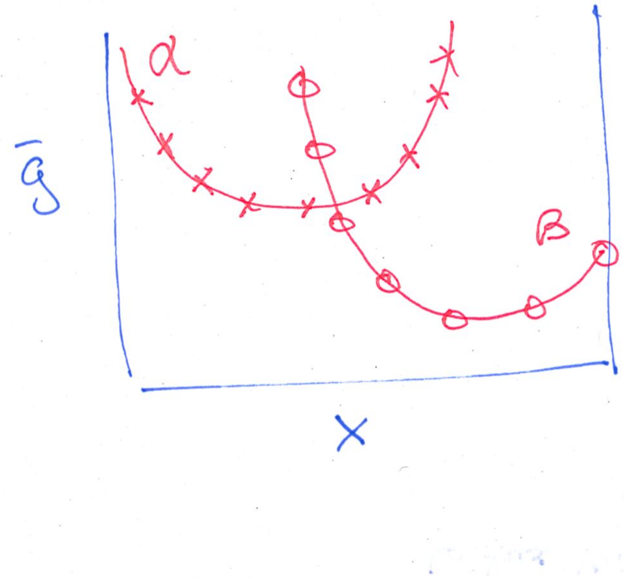
c={A,B}

$\bar g'_\varepsilon = \mu_A^{\beta+\delta}X_A^\varepsilon + \mu_B^{\beta+\delta}X_B^\varepsilon$

if $\bar g'_\varepsilon > \bar g_\varepsilon \Rightarrow$ then β+δ is metastable relative to ε ⇒ ~~β~~ is known to be stable so try β+ε and repeat

→ filter for composition if desired.

phases with variable composition



lecture 10.4 2021

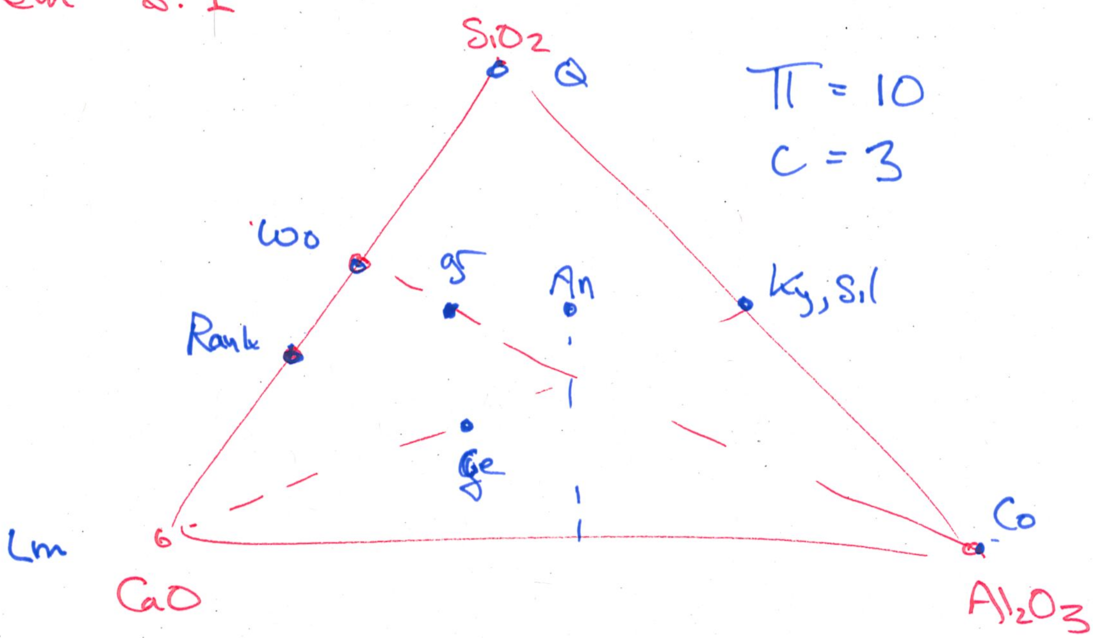
LP → simplex → slow → only robust solution

LP → interior points → iterative

Kantorovich → road of life, '41 - '44 → formulated. → NPE '75

Dantzig → simplex ~ ww II. → solved.

Problem 6.1



$\Pi = 10$

$C = 3$

Chapter 7 problem 7.1 only!!