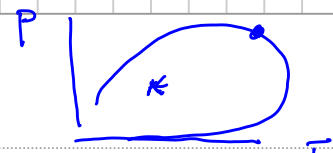


PHASE EQUILIBRIA CALCULATIONS

Note Title

2/3/2017



* COMPONENT PARTITIONING - K-values ($K_i = \frac{y_i}{x_i}$)

* PHASE SPLIT CALCULATIONS
($n_g | n_o, m_g | m_o, V_g | V_o$)
 $y_i \quad x_i$

FLASH @ (P, T)
Saturation Pressure @ T

* PHASE PROPERTIES (ρ, μ, σ)

Volumetric
Transport
Inter-phase

- Direct lab measurement (Ch. 6)
- Estimate / calculate by Correlation / EOS
Ch. 3 \neq 4 (\neq 5)

PROBLEM 2

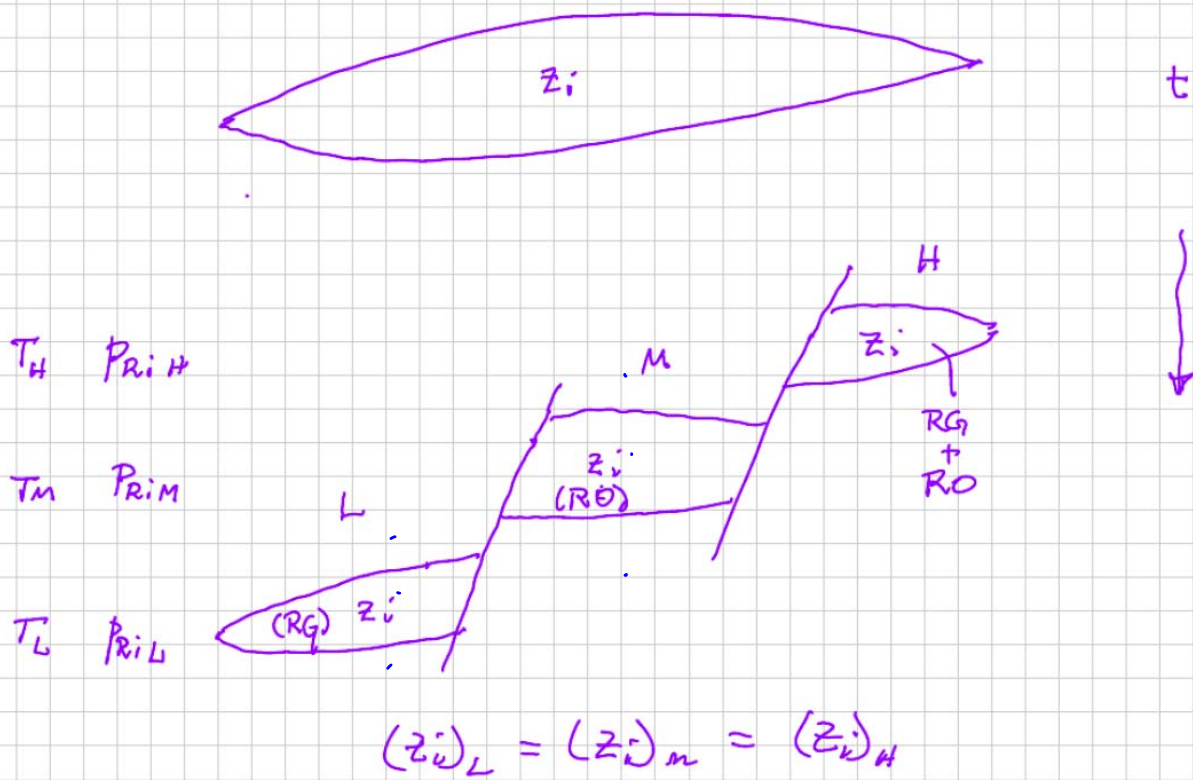
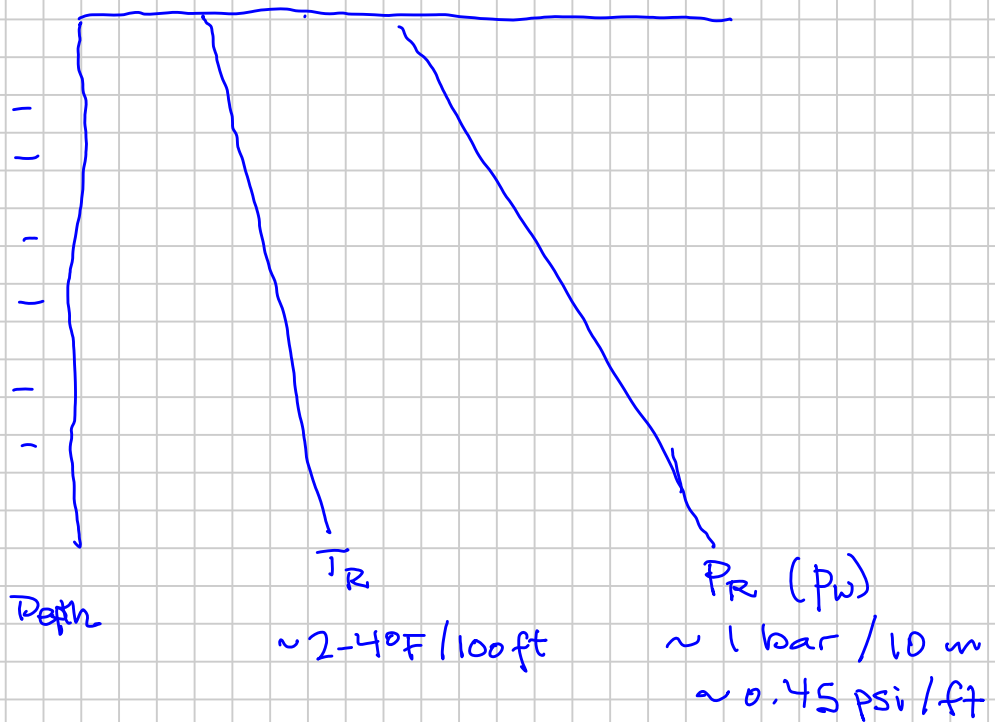


Fig. 1 – Sketch of reservoir, originally (above) and after faulting (below).



$\frac{D}{(ft)}$ $\frac{P}{(psia)}$ $\frac{T}{(°F)}$

5300 2650 160
 ↓ ↓
 6900 3450 192

$$\Delta T = 32^\circ F \Rightarrow \Delta D = 32^\circ F \cdot \frac{100 \text{ ft}}{2^\circ F}$$

$$= 1600 \text{ ft}$$

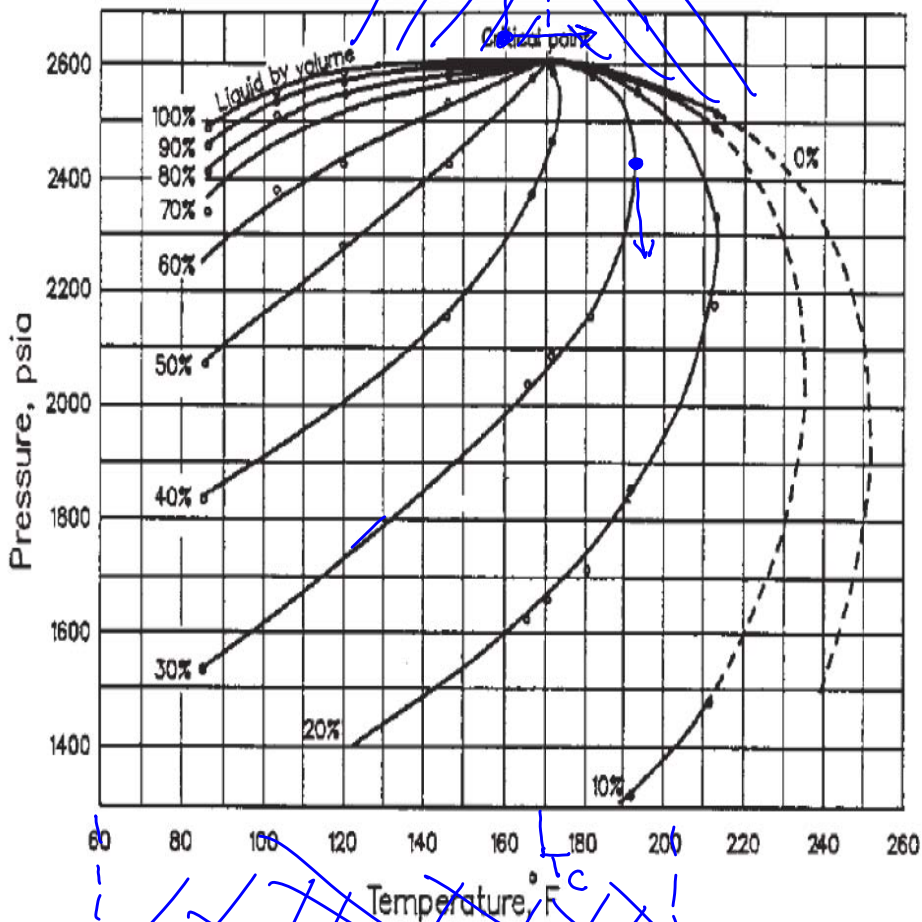
$$\frac{5300}{16900}$$

$$\Delta p = \Delta D \cdot \frac{\Delta P}{\Delta D}$$

$$= 1600 (0.5)$$

$$= 800 \text{ psi}$$

$$\frac{2650}{3450 \text{ psia}}$$



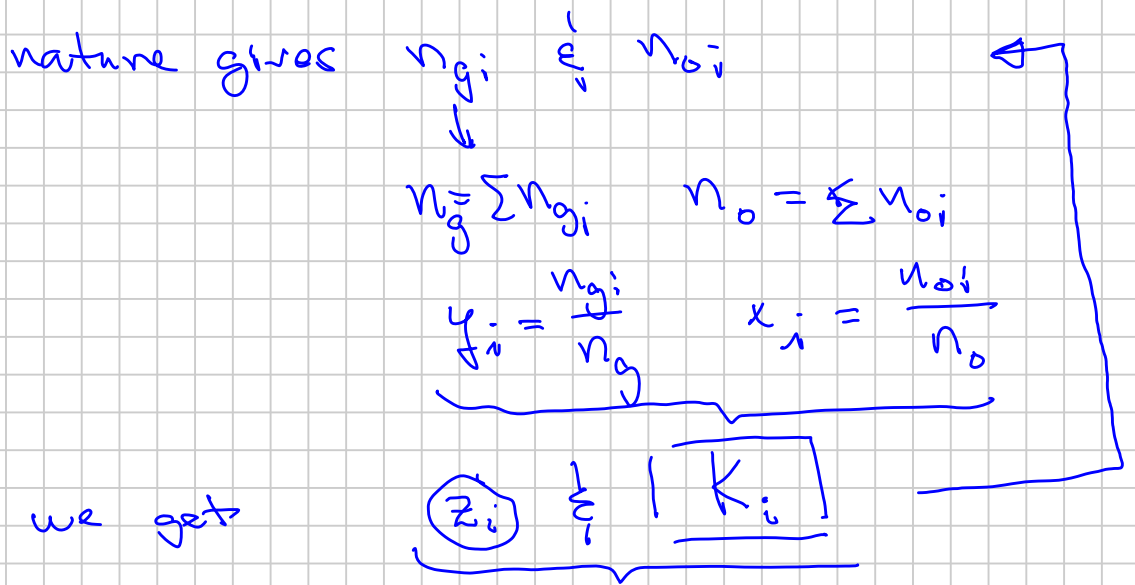
$k_i \approx \frac{P_{oi}(T)}{P}$

* Component Partitioning of mixture z_i @ (p, T)

How mother nature decides how many of the moles of i ($n_i = n \cdot z_i$) partitions into the gas phase ($n_{gi} = n_g y_i$) and into the oil phase ($n_{oi} = n_o \cdot x_i$)

K-value

Definition of Equilibrium Ratio $K_i \equiv \frac{y_i}{x_i}$



We know lots about $K_i(p, T)$

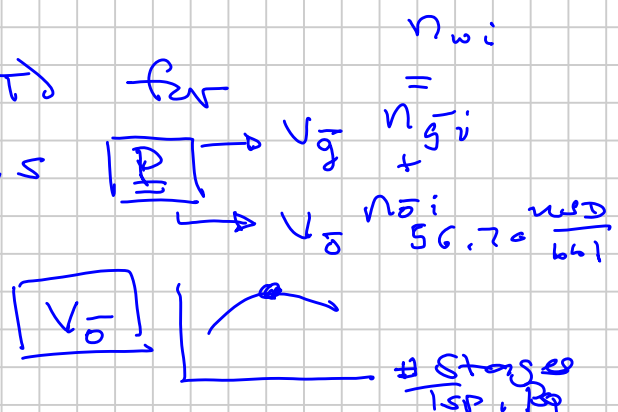
$p \approx 50-100$ bar

Any oil & gas field in the world

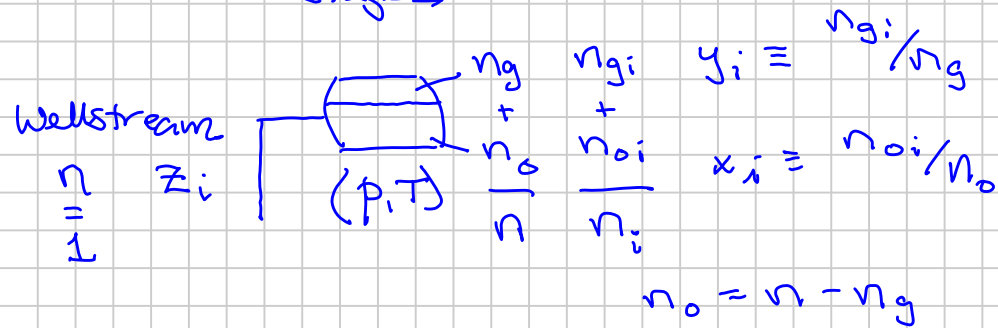
$$z_i K_i \approx \frac{p_{vi}(T)}{p}$$

Reasonably valid $K_i(p, T)$ for Surface Process Calculations

Muskat & McDowell



Stage 1



Component M.B. $z_i n = y_i n_g + x_i n_o + x_i (n - n_g)$

Divide by n

$$z_i = y_i \frac{n_g}{n} + x_i \left(1 - \frac{n_g}{n}\right)$$

Define $f_g \equiv \frac{n_g}{n}$

Know: $\frac{y_i}{x_i} = K_i(p, T) = \frac{P_{ri}(T)}{p}$

$$z_i = y_i f_g + x_i (1 - f_g)$$

Want to know: f_g, y_i, x_i

$$S_o \frac{V_o}{V_o + V_g} = \frac{1}{1 + \frac{V_g}{V_o}}$$

$$\frac{V_g}{V_o} = \frac{f_g (M/P)_g}{(1 - f_g) (M/P)_o}$$

Volume Ratio

$$z_i = y_i f_g + x_i (1 - f_g)$$

$$K_i = y_i / x_i \quad y_i = K_i x_i$$

$$z_i = K_i x_i f_g + x_i - x_i f_g$$

$$= (k_i - 1)x_i f_g + x_i$$

$$z_i = x_i [(k_i - 1)f_g + 1]$$

Once f_g found

$$\left\{ \begin{array}{l} x_i = \frac{z_i}{(k_i - 1)f_g + 1} \\ y_i = k_i x_i = \frac{z_i k_i}{(k_i - 1)f_g + 1} \end{array} \right\} \begin{array}{l} \text{know } z_i \\ k_i \\ \text{Don't know } f_g \end{array}$$

$\sum z_i = 1$ known
therefore

$$\underbrace{\sum y_i = 1 \quad \sum x_i = 1}_{\text{Must be}}$$

$$\underline{\underline{\sum y_i - \sum x_i = 0 = \sum (y_i - x_i) = h(f_g)}}$$

$$h(f_g) = \sum \frac{z_i k_i}{(k_i - 1)f_g + 1} - \frac{z_i}{(k_i - 1)f_g + 1}$$

$$h(f_g) = \sum \frac{z_i (k_i - 1)}{(k_i - 1)f_g + 1} = 0$$

Rachford-Rice Equation 1952 (Syn after 1949)

Muskat-McDowell

$$c_i \equiv \frac{1}{k_i - 1} \quad c_i = 0 \text{ , if } k_i = 1$$

$$\boxed{h(f_g) = \sum_{T_i} \left(\frac{z_i}{f_g + c_i} \right) = 0}$$

know k_i , z_i @ (P,T)
(est)

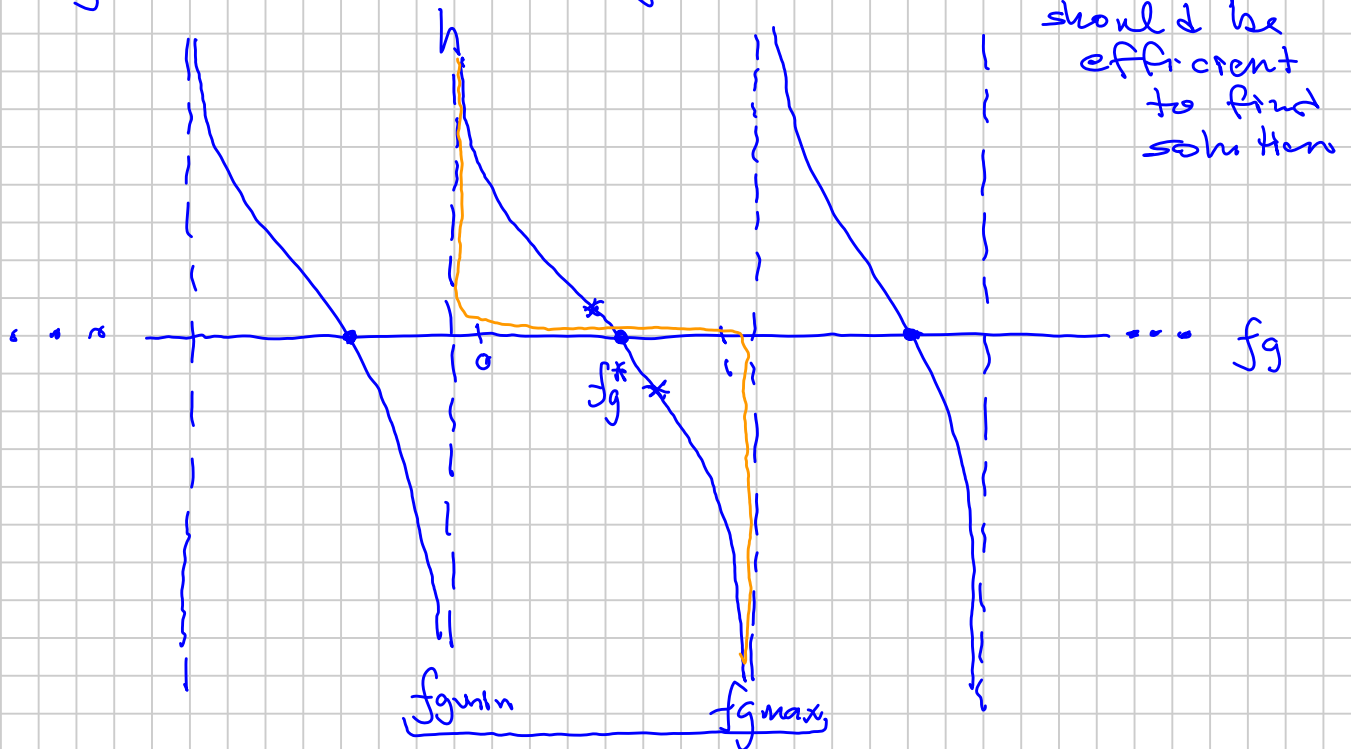
Characteristics of the MM (ICR) equation:

1. The ^{physically} correct f_g solution guarantees physical consistency ($x_i \geq 0$, $y_i \geq 0$) is

$$f_{gmin} < f_g^* < f_{gmax}$$
$$= \frac{1}{1 - K_{max}} \qquad = \frac{1}{1 - K_{min}}$$

where $K_{max} > 1$
 $K_{min} < 1$ } if not, NO 2-phase split

2. $h(f_g)$ is a monotonic function \Rightarrow Newton-Raphson



3. $f_{gmin} \leq 0 < 1 \leq f_{gmax}$

Practical Application:

$$\underline{i} \quad \underline{z_i} \quad \underline{K_i(P,T)} \quad \underline{c_i} \quad \underline{T_i} \quad \underline{y_i} \quad \underline{x_i} \quad \frac{\boxed{f_g}}{\boxed{h}} = \sum T_i$$

$$\underline{1} \quad \underline{1} \quad \underline{1}$$

Equilibrium Ratios (K-values) Estimation & General Behavior

① Low-pressure range: $K_i \approx \frac{P_{vi}(T)}{P}$

Ch. 3 Wilson Eq. (using a correlation by Edmister for $P_{vi}(T)$)

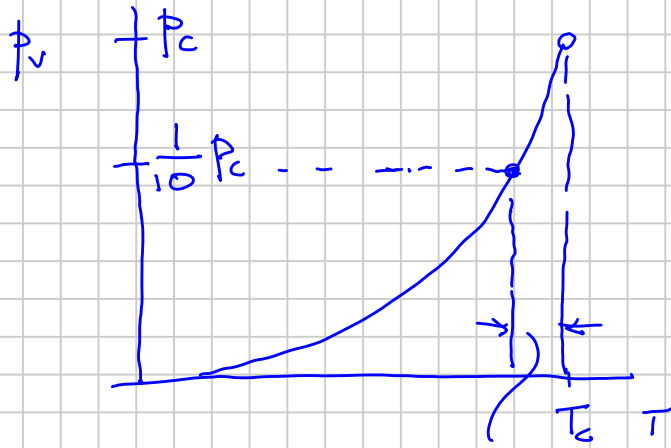
$$K_i = \frac{\exp\left[5.37(1 + \omega_i)\left(1 - T_{ri}^{-1}\right)\right]}{P_{ri}}, \dots \dots \dots (3.157)$$

$$T_{ri} = \frac{T}{T_{ci}} \quad \text{absolute units (K, } ^\circ\text{R)}$$

$$\phi_{ri} = \frac{P}{P_{ci}}$$

ω_i known physical quantity for all components (0-1)

Pitzer



30% drop in T

(0.7 T_c)

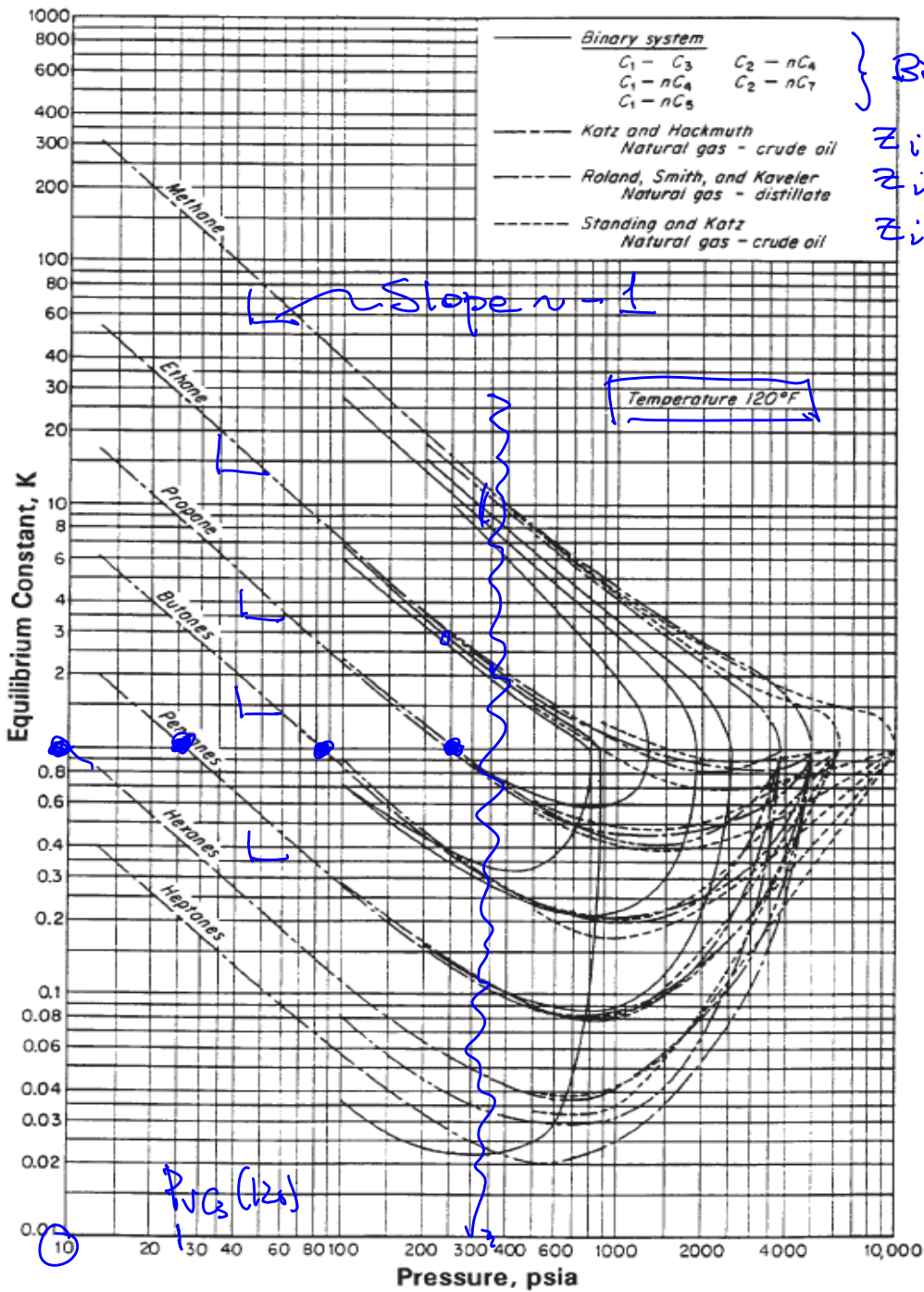
$$\omega \equiv -1 - \log_{10} \left(\frac{p_v(0.7 T_c)}{p_c} \right)$$

0

~0.1 simple compounds
C, He...

1

$$0.01 = \frac{1}{100}$$



Binaries

Z_i
 Z_i
 Z_i

$$K_i = \frac{P_{vi}}{p}$$

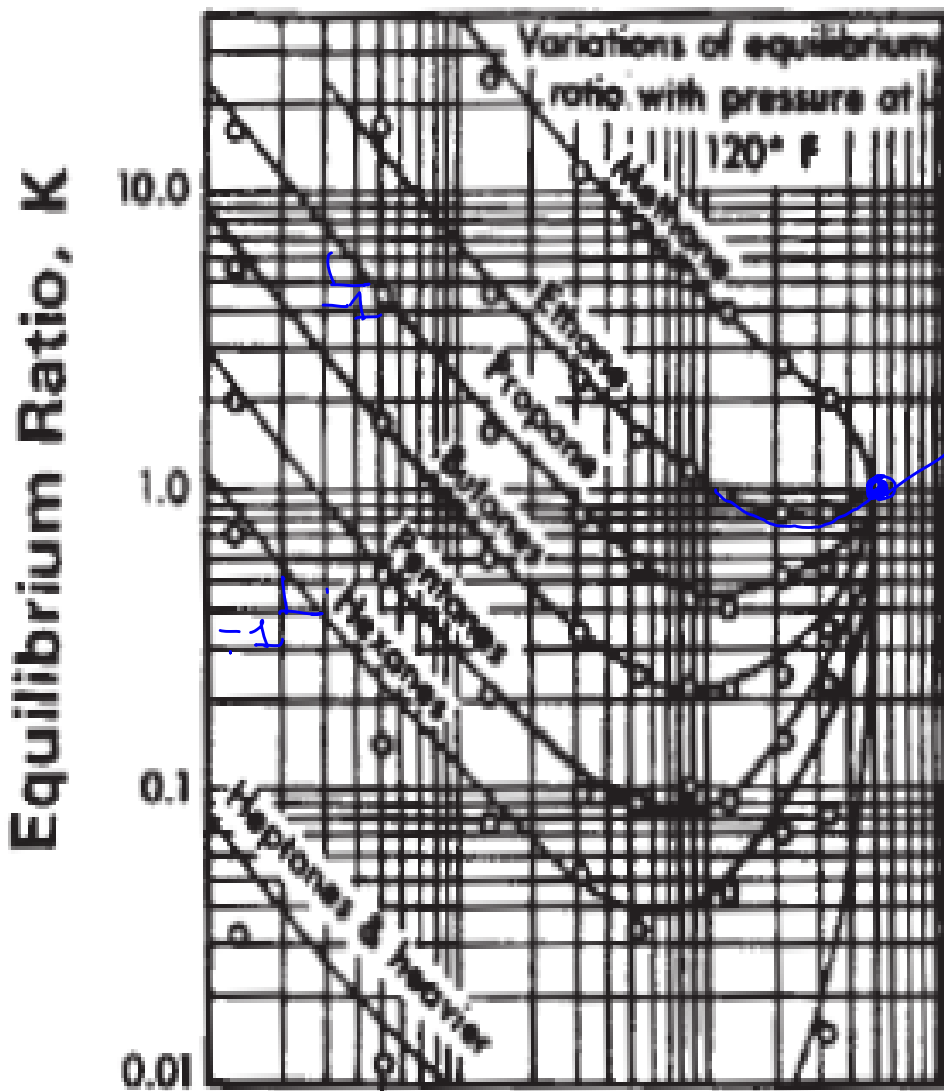
$$\log K_i =$$

$$\log P_{vi} - \log p$$

$$K_i = 1$$

$$0 = \log P_{vi} - \log p$$

$$p = P_{vi} \text{ when } K_i = 1$$



Given z_i
 $N_2 \& C_1$
 nonatonic
 approach to 1
 @ P_K
 (2)
 At same
 high pressure
 all K_i
 converge
 together to
 $K_i = 1$

Apparent
 Convergence
 Pressure, $\left[\frac{p}{p_K} \right]$

Vary

$$p_K(T, z_i)$$

1983 (85) Modified
 Wilson Eq.

Whitson and Torp¹⁰⁰ suggest a generalized form of the Hoffman *et al.*⁹⁹ equation in terms of convergence pressure and acentric factor.

$$K_i = \left(\frac{p_{ci}}{p_K} \right)^{A_1 - 1} \frac{\exp \left[5.37 (A_1) (1 + \omega_i) \left(1 - T_{ri}^{-1} \right) \right]}{p_{ri}}, \quad (3.159)$$

where A_1 = a function of pressure, with $A_1 = 1$ at $p = p_{sc}$ and $A_1 = 0$ at $p = p_K$. The key characteristics of K values vs. pressure

$$A_1(p) = 1 - \left(\frac{p}{p_K} \right)^{A_2} \rightarrow 0.5 - 0.8$$

$$A_1 = 1 - (p/p_K)^{A_2}, \quad (3.160)$$

where A_2 ranges from 0.5 to 0.8 and pressures p and p_K are given in psig. Canfield¹⁰⁵ also suggests a simple K -value correlation based on convergence pressure.

