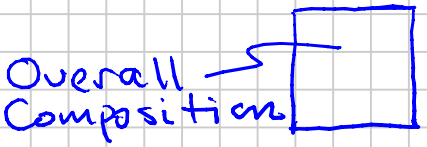
Isothermal Flash Calculation (Rachford-Rice)

Note Title 2012-09-21

Problem Statement: (1) How many phases (V L): 1 or 2 (0 or 1)

- Under-saturated
- Saturated: 2 phases ($1-\epsilon$ ϵ)



(p, T) Fixed, Known, Specified

(2) How much of each phase (moles or mole fraction)

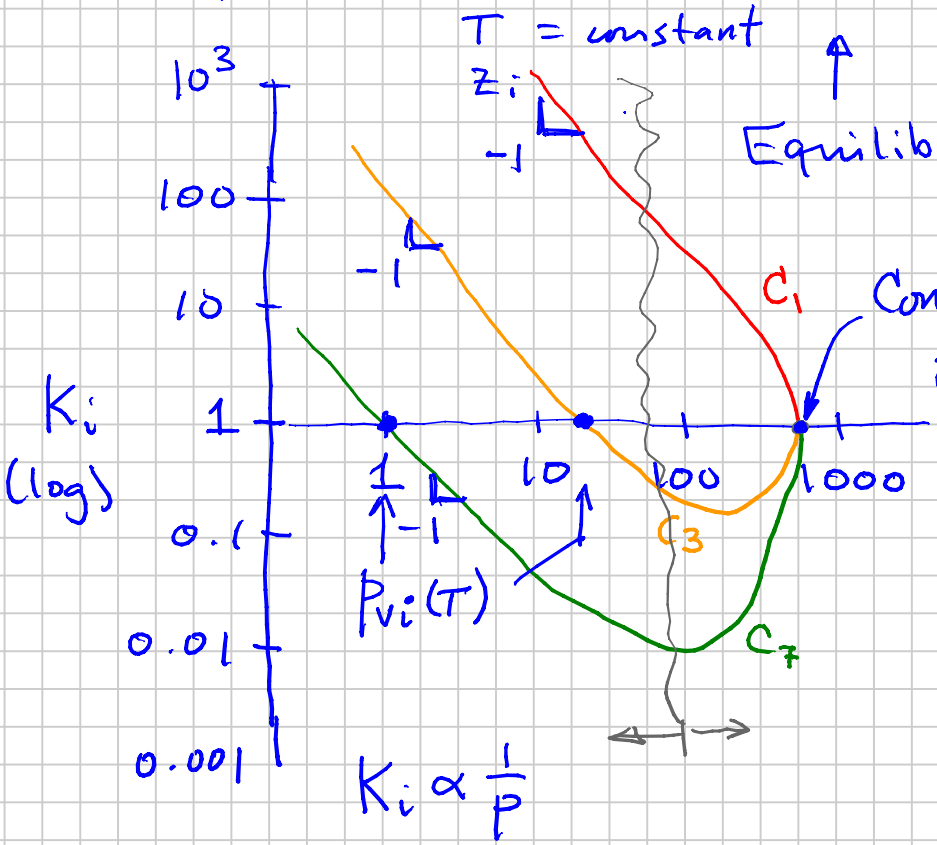
n_V / n_L $\qquad f_V \equiv \frac{n_V}{n}$

(3) Molar composition of each phase V: y_i

L: x_i

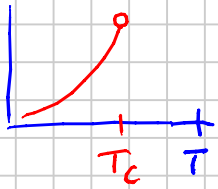
Solution:

Requires estimate of $K_i = \frac{y_i}{x_i}$ @ (p, T, z_i)



$K_i \propto \frac{1}{p}$

Equilibrium Ratio



Convergence Pressure p_k

$K_i \to 1$

$p_{(log)}$ [bara]

$p_k(T, z)$

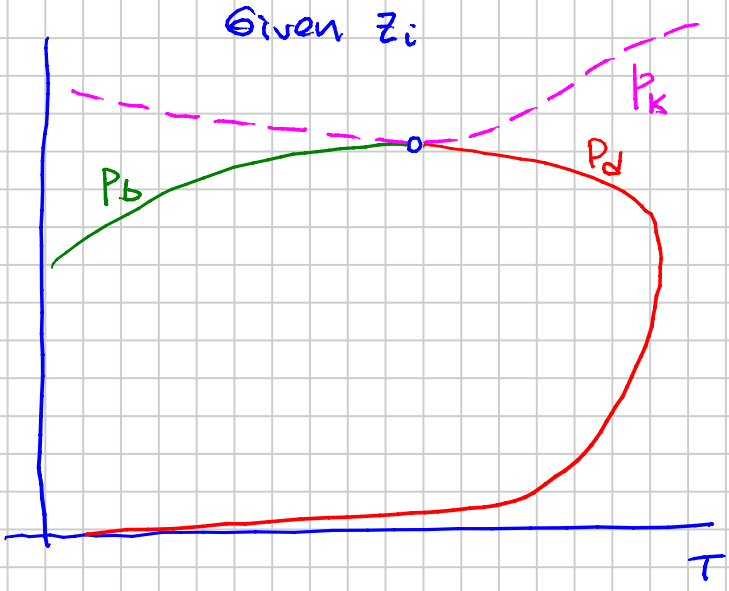
If $T = T_c$ of z_i

$\Rightarrow p_k = p_c$ of z_i

SPE PBM

*Modified Wilson Eq.

$$K_i \left(p, T, p_K ; \underset{=}{p_{ci}}, \underset{=}{T_{ci}}, \underset{=}{\omega_i} \right)$$



Component Material Balance:

$$\begin{cases} n_i = n_{Li} + n_{vi} \\ \text{Total Material Balance} \\ n = n_L + n_v \end{cases}$$

$$n = \sum_{i=1}^{N} n_i \qquad n_L = \sum_{i=1}^{N} n_{Li} \qquad n_v = \sum_{i=1}^{N} n_{vi}$$

Define:

$$z_i \equiv \frac{n_i}{n} \qquad y_i \equiv \frac{n_{vi}}{n_v} \qquad x_i \equiv \frac{n_{Li}}{n_L}$$

$$f_v \equiv \frac{n_v}{n} \quad ; \quad f_L = \frac{n_L}{n} = 1 - f_v$$

Also show:

$$\sum z_i = 1 = \sum y_i = \sum x_i$$

$$K_i \equiv \frac{y_i}{x_i} \qquad \text{know}$$

$$\left.\begin{array}{l} \boxed{z_i = f_v y_i + (1-f_v) x_i} \\ n_i = n_{vi} + n_{Li} \end{array}\right\} \text{same thing}$$

$$K_i = y_i / x_i$$

$$\rightarrow \quad y_i = K_i x_i$$

$$z_i = f_v \cdot (K_i x_i) + (1 - f_v)\, x_i$$

Solve this for x_i

$$z_i = x_i \left[f_v K_i + (1 - f_v) \right]$$

$$z_i = x_i \left[f_v (K_i - 1) + 1 \right]$$

$$x_i = \frac{z_i}{f_v (K_i - 1) + 1}$$

$$y_i = K_i x_i = \frac{z_i K_i}{f_v (K_i - 1) + 1}$$

1949 : Muskat - McDowell

$$\Sigma y_i = 1 \qquad \Sigma x_i = 1$$

$$\Sigma y_i - \Sigma x_i = 1 - 1 = 0$$

$$\sum_{i=1}^{N} (y_i - x_i) = 0$$

"Rachford-Rice": 195x

$$h(f_v) \equiv \sum_{i=1}^{N} \left[\frac{z_i (K_i - 1)}{f_v (K_i - 1) + 1} \right] = 0 \qquad (1)$$

if $f_v = \dfrac{-1}{K_i - 1}$

1949 : M-M

$$c_i \equiv \frac{1}{K_i - 1} \quad ; \quad c_i = 0 \text{ if } K_i = 1$$

$$h(f_v) = \sum_{i=1}^{N} \left[\frac{z_i}{f_v + c_i} \right] = 0 \qquad (1')$$

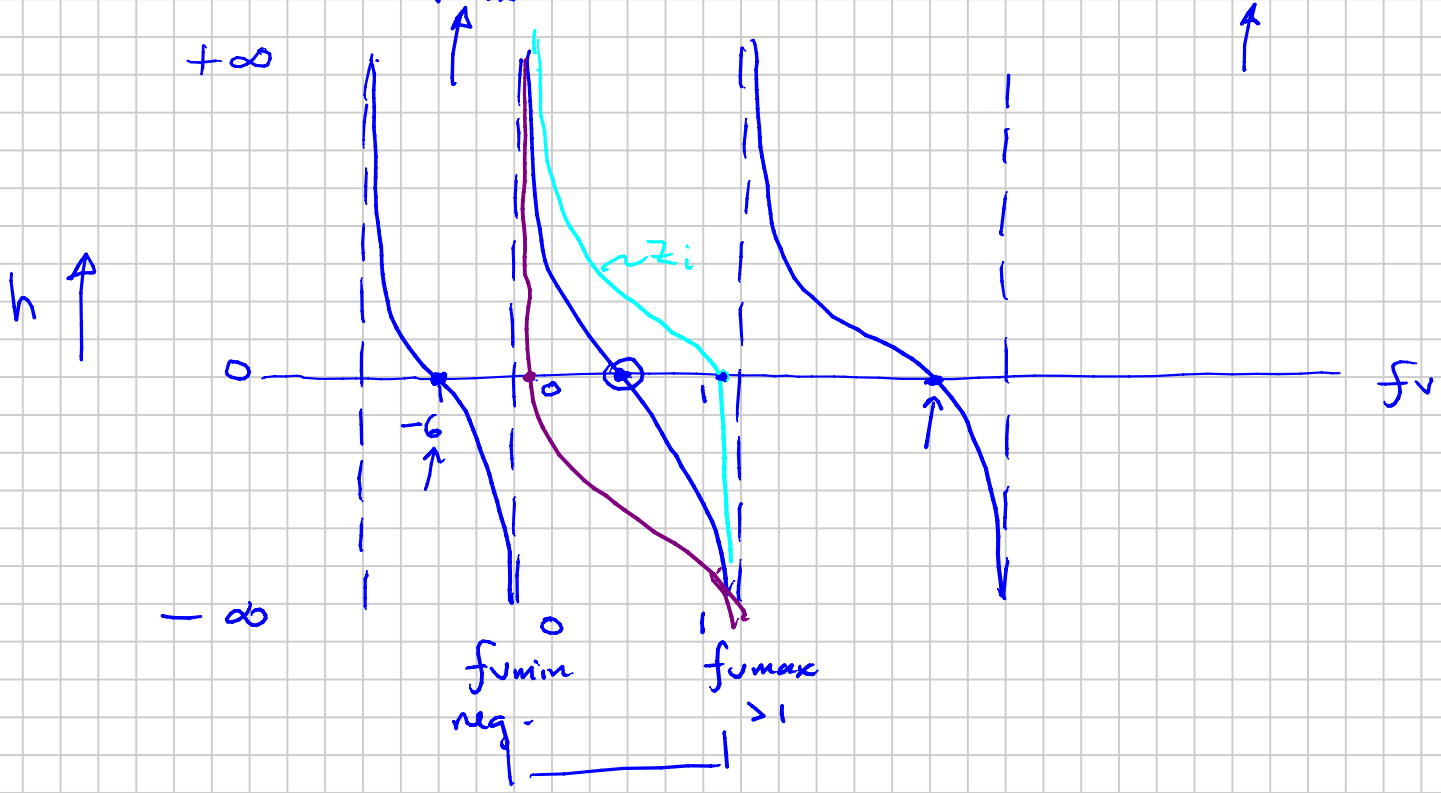
(1) $h(f_v)$ is a monotonic function → NR

(2) N-1 solutions

- Only one of these yields physical solution

$$x_i \geq 0, \quad y_i \geq 0$$

$$0 > \frac{1}{1-K_{max}} = f_{v\,min} < f_v < f_{v\,max} = \frac{1}{1-K_{min}} > 1$$



: Solved f_v^*

L + V $\quad 0 < f_v^* < 1$: two phase solution

Liquid $\quad f_v^* = 0$
Vapor $\quad f_v^* = 1$
} : saturated single phase

Liquid-Like $\quad f_v^* < 0$
Vapor-Like $\quad f_v^* > 1$
} : undersaturated single phase

<1% of calculations ...

$z_i \to \epsilon$

$K_i \to \epsilon$ or huge

Setup for Solution:

P, T, z_i Given

Guestimate
Estimate

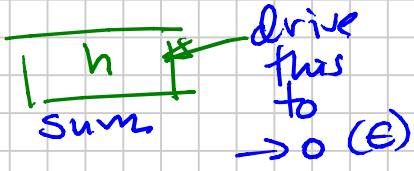
1. Estimate $K_i(P, T, p_K)$: Wilson Ch. 3 or 4

2. Setup a Table

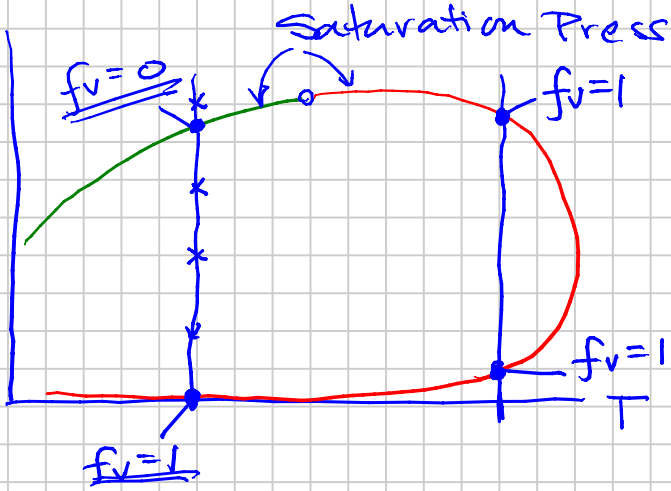
Guess: fv

Calc: fvmin, fvmax

i	z_i	K_i	$C_i = \frac{1}{K_i - 1}$	$Term_i$	y_i	x_i
1						
2		K_{max}				
⋮						
N		K_{min}				



Special Cases of Flash Calculation:



$f_v = 0$: Bubblepoint

$f_v = 1$: Dewpoint

Bubblepoint : $f_v = 0$ "Bubble"

$\Rightarrow \sum y_i = 1$ equation

$$h_{BP}(p_b) = 1 - \sum_{i=1}^{N} z_i (K_i(p_b)) = 0$$

$y_i = x_i K_i$

$y_i = z_i K_i (p ; \underbrace{T, p_K}_{\text{fixed}})$

search

Dewpoint: x_i $f_v = 1 - \epsilon$

ϵ phase

$\sum x_i = 1$

$x_i = y_i / K_i$

$x_i = z_i / K_i (p ; T, p_K)$

z

Fixed T, p_K

$$h_{DP} = 1 - \sum x_i = 0 = 1 - \sum \frac{z_i}{K_i(p)}$$

Two Solutions:

Upper DP

Lower DP