Note Title 2/6/2018

FLASH Calculations : Q's & Review

Knowing: $z_i \quad (p, T) \Rightarrow K_i \equiv \dfrac{y_i}{x_i}$ (est. or known)

Unknown: $y_i \quad x_i \quad , \quad f_v \equiv \dfrac{n_v}{n_v + n_L} = \dfrac{n_v}{n}$

Solve $\underbrace{h(f_v)}_{\text{monotonic}} = \sum y_i - x_i = \sum \dfrac{z_i (K_i - 1)}{1 + f_v (K_i - 1)} = 0$ (RR)

$\dfrac{1}{1-K_{max}} = \underline{f_{v_{min}}} < f_v < \underline{f_{v_{max}}} = \dfrac{1}{1-K_{min}}$

N-1 solutions

One guarantees $y_i \geq 0, \; x_i \geq 0$

$\sum \dfrac{z_i}{c_i + f_v}$ (MM)

$c_i \equiv \dfrac{1}{K_i - 1}$

N

Calc: $y_i =$, $x_i =$ } from z_i, K_i, f_v

$(z_i = x_i)$ Bubblepoint

Dewpoint $(z_i = y_i)$

$\boxed{\text{Physically}}$: $0 \leq f_v \leq 1$

$f_{v_{min}} < 0 \leq f_v \leq 1 < f_{v_{max}}$

{ If $K_{min} < 1$ & $K_{max} > 1$ } requirement for any solution

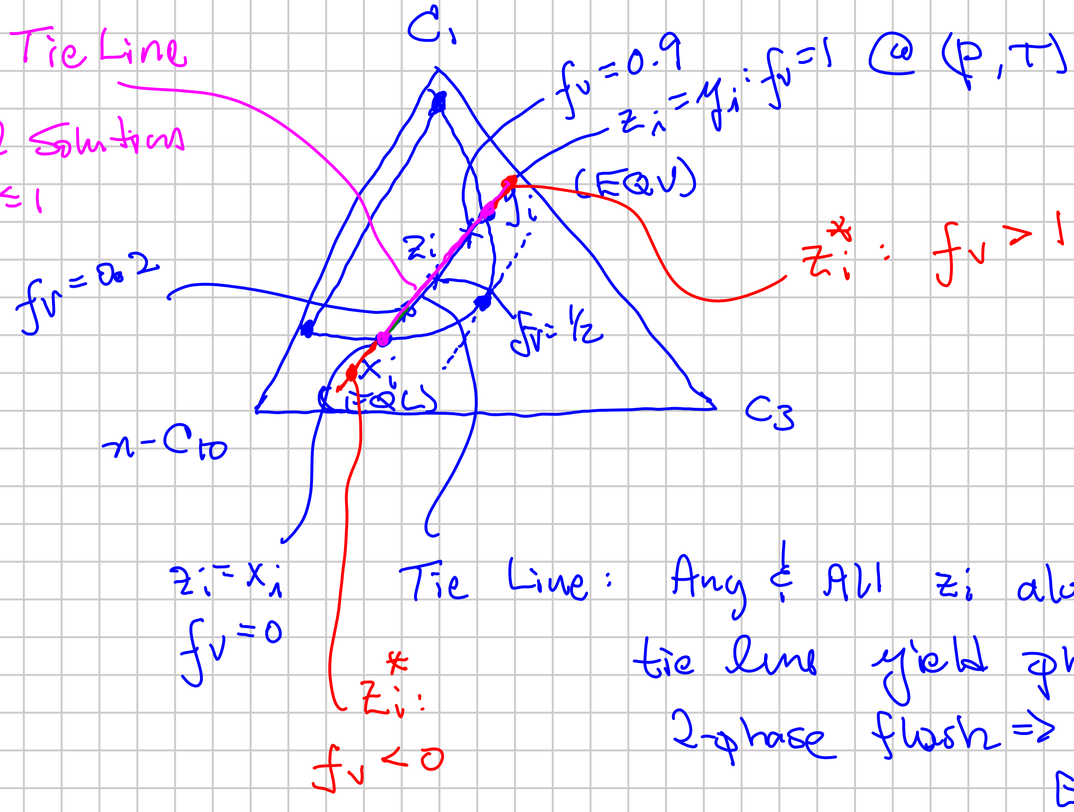
$\boxed{\text{Mathematically}}$: May be useful "Negative Flash"

$\underbrace{f_v < 0 \text{ or } f_v > 1}_{\text{non-Physical Phase Amount } (<0)}$ still $\underbrace{y_i > 0 \qquad x_i > 0}_{\text{Physical Equilibrium Solution}}$

X

(*)

Pink: Tie Line
⇒ Physical Solution $0 \le f_v \le 1$

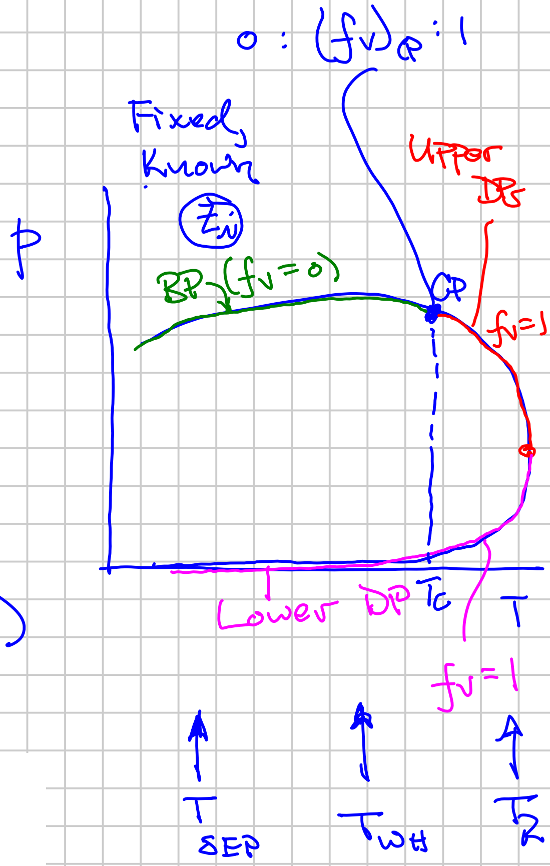


Tie Line: Any & All z_i along the tie line yield physical 2-phase flash ⇒ y_i EQV, x_i EQL

Saturation Pressure Calculation

- Compute p_s @ T

Type: BP
DP (upper)
DP (lower)



- Know: $\{z_i, T\}$; Equation $K_i(\underline{\underline{p}} ; @T, z_i)$

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

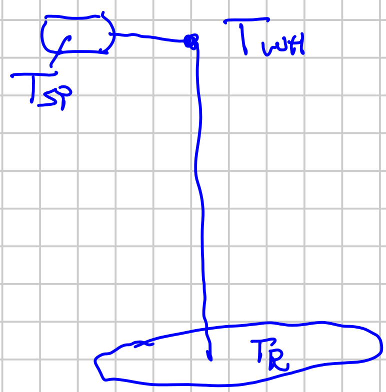
(p, p, T^*, p)

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

and temperature are correctly predicted by Eq. 3.159, where the following pressure dependence for A_1 is suggested.

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

where A_2 ranges from 0.5 to 0.8 and pressures p and p_K are given



Given: z_i^*, T^*, $K_i(p; T, z_i^*)$

Solve: p_s @ T^*

"S": BP, DP

$\boxed{p_b}$ BP: (1) $x_i = z_i$ $\quad f_v = 0$

$$z_i = \underbrace{f_v \, y_i} + (1-f_v)\, x_i$$

(2) . y_i don't know ⇒ solve

$\sum y_i = 1$ constraint eq.

(3) $K_i = \dfrac{y_i}{x_i} = \dfrac{y_i}{z_i}$

$$y_i = z_i K_i$$

$$\sum y_i = 1 = \sum z_i K_i$$

Bubblepoint Calculation

$$\boxed{h_{BP}(p_b) = 1 - \sum z_i \underbrace{K_i(p)}_{@T^*,\, z_i^*} = 0}$$

Dewpoint:

(1) $y_i = z_i$ $\quad f_v = 1$

(2) x_i ? $\quad \sum x_i = 1$

③ $K_i = \frac{y_i}{x_i} = \frac{z_i}{x_i}$

$\Rightarrow x_i = z_i / K_i$

$\sum x_i = 1 = \sum z_i / K_i$

Dewpoint: $\boxed{h_{DP}(p_d) = 0 = 1 - \sum z_i / K_i(p)}$

May be two physical solutions at T^*

Upper DP : p_{du}

Lower DP : p_{dL}

General Cautions:

Use Modified Wilson Eq. $K_i(p, T, p_K, \theta_i)$

$(T_{ci}\ p_{ci}\ \omega_i)$

$p = p_K \Rightarrow K_i = 1$

$p_d = p_K \Rightarrow h_{DP} = 0$

$p_b = p_K \Rightarrow h_{BP} = 0$

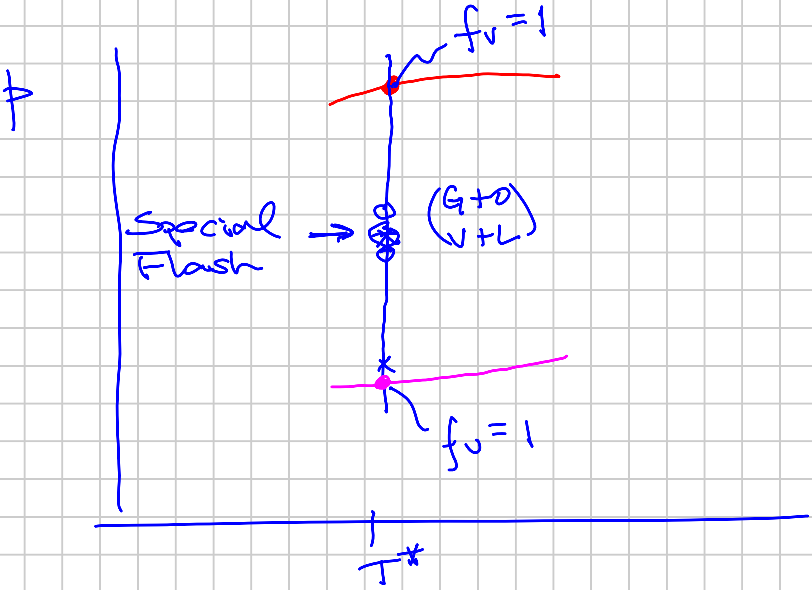
Usually be the WRONG solution "trivial"

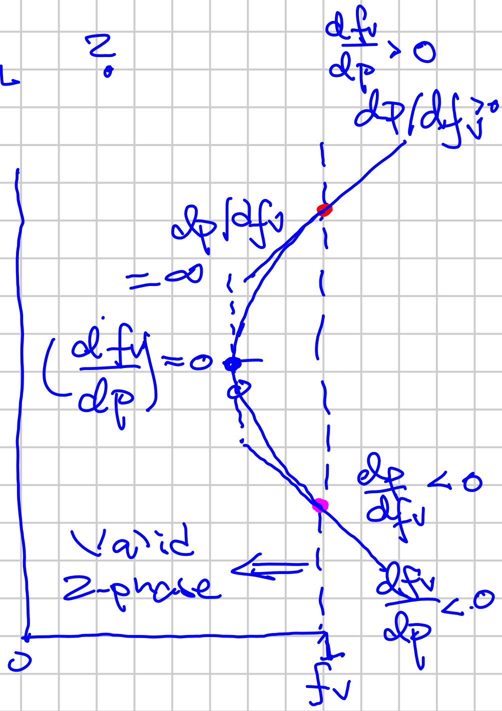
If $T^* = T_c$ $\quad p_s = p_b = p_d = p_K$ Valid Solution

You don't T_c ?

BP or Upper DP ?

How to force search p_{dw} vs p_{dr} ?





$h_{BP}(p)$ $\underbrace{= 0 \ @ \ p_b}$

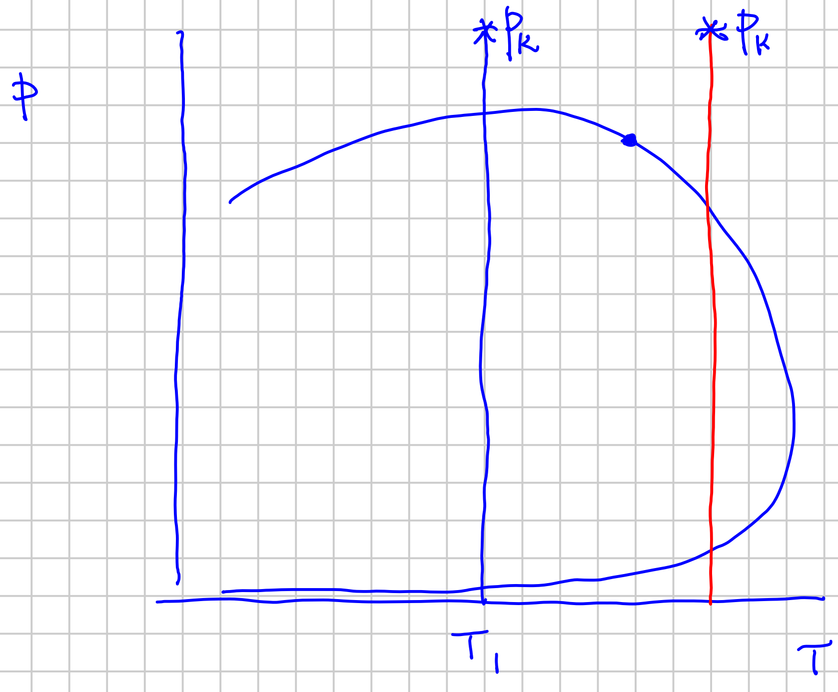
$h_{DP}(p)$ $\underbrace{= 0 \ @ \ p_d}$

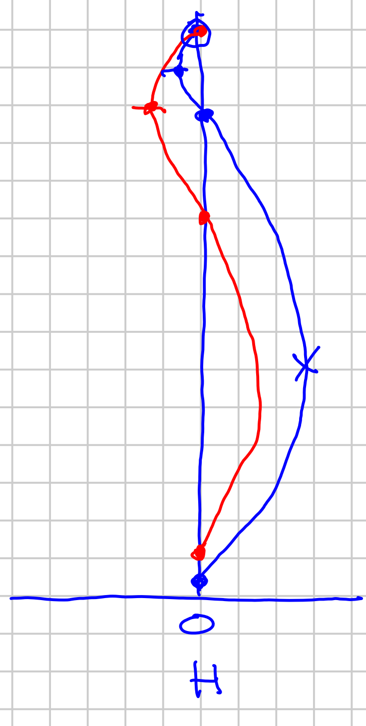
$\cancel{H_1 = h_{BP}^2 + h_{DP}^2}$

$H_2 = h_{BP} \cdot h_{DP}$

Solve ~~H_1 or~~ $H_2 = 0$

Then ask what kind of p_s





Upper Sat. Pressure $\quad H \geq 0$