



- Allocated rates (Daily)
  - well Tests + Metering
- Reservoir Simulation
  - using same  $\underline{P}$  ( $q_g, q_o$ )

## \* Unit Flash Calculations

### P-T Flash

- $z_i \rightarrow$  Entering the Unit
- $p, T$  specified
- $K_i(p, T, z_i) \equiv \frac{y_i}{x_i}$ 
  - Correlations (modified Wilson)
  - Trial-and-Error w/ EOS
- Thermodynamic Consistency

$$\left. \begin{array}{l} \mu_{vi} = \mu_{Li} \\ \mu_{gi} = \mu_{oi} \end{array} \right\} \begin{array}{l} \underline{\text{EOS}}: \\ \text{Equal} \\ \text{Chemical} \\ \text{Energy} \end{array}$$

EQUATION OF STATE (EOS) - Gases & oils

(1) Name: SRK (Soave Redlich Kwong)  
PR (Peng Robinson)

(2) Table 1 - Component Properties

<u>Name</u>	{ $p_c$	$T_c$	$\omega$ }	$M$	$S(C)$	
$N_2$						
$CO_2$						
$H_2S$						
					Volume Shift (instead of COSTALD)	Rackett

(3) Table 2 - Binary Interaction Parameters (BIPs)  $k_{ij} \sim -0.1$ -ish to  $+0.2$ -ish

$N_2$   $CO_2$   $H_2S$   $C_1$  ...

$N_2$

$CO_2$

$H_2S$

$C_1$

...

$k_{ii} = 0$

Diagonal

$k_{ij} = k_{ji}$

Symmetric

$CO_2-HC$

$N_2-HC$

$H_2S-HC$

Defaults:

$\sim 0.05-0.15$

Bit different SRK & PR

SRK HC-HC

$\sim 0$

default

PR HC-HC

$\sim 0$

default

EXCEPT  $k_{C_1-C_7+} \sim 0.02-0.1$

( $\geq 50-100$  bara)

$k_{ij}$  Affect

$K_i$  &  $K_j$

at

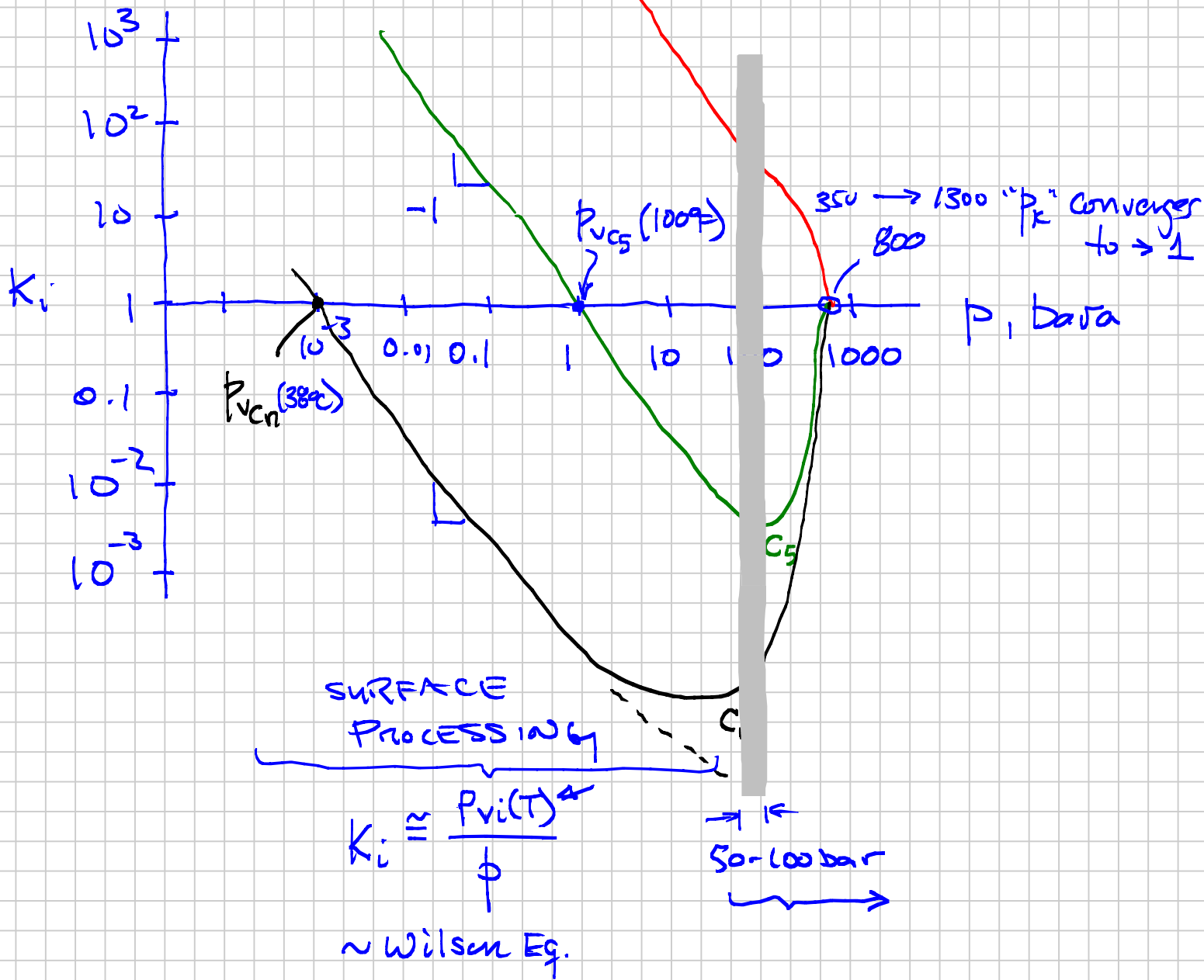
higher pressures

⚠ Near Critical Points

PRIMARILY

# K-Value Behavior

T = Fixed = 100°F  
38°C



$K_i \sim f(P_i, T)$   
NOT  $z_i$

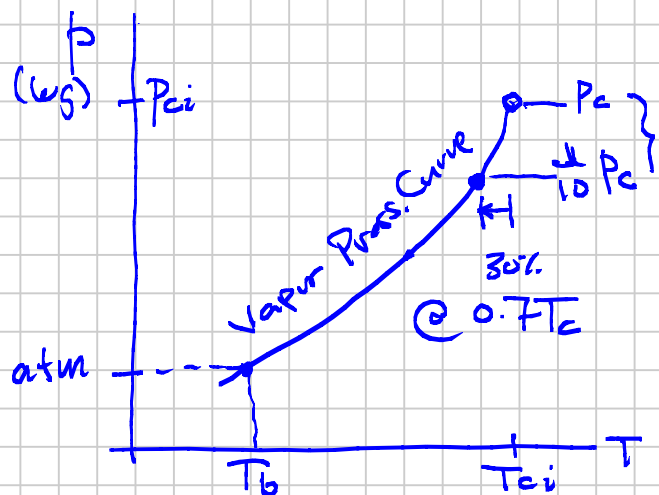
$K_i(P_i, T, z_i)$

$K_i^{EOS}(P_i, T, z_i; \underline{\underline{BIPs}})$

EOS (Table 1):  $T_c, P_c, \omega_i$

Component  $i$

Normal Pressure ⇒



Pitzer :  $\omega \equiv -1 - \log_{10} \frac{P_v(0.7T_c)}{P_c}$

He  
 $\omega_1 = -1 - (-1) = 0$

C<sub>40</sub>  $\frac{P_v(0.7T_c)}{P_c} \sim \frac{1}{100} \Rightarrow \omega \sim 1$

$\omega_i$  (with  $T_c, P_c$ )  $\Rightarrow$  guaranteed EOS (PR or SRK)

gives ACCURATE  $p_{vi}(T)$

$\Rightarrow$  ACCURATE  $K_i(T, p \leq 100 \text{ bar})$

M SRK

EOS: 
$$p = \frac{RT}{v-b} - \frac{a \cdot \alpha_{SRK}(T, \omega)}{v(v+b)}$$

Given  $x_i$ :  
 $a_i, b_i, P_i, T_i$

$\omega_i$

$\boxed{v}$

$v \equiv \frac{V}{z}$

$\sqrt{p} = \frac{M}{\sqrt{V}} = \frac{m}{\sqrt{V}}$

$a = \Omega_a \frac{R^2 T_c^2}{P_c}$        $\Omega_a \approx 0.4$

$b = \Omega_b \frac{RT_c}{P_c}$        $\Omega_b \approx 0.1$

$$\alpha_i = \left[ 1 + m_i (1 - \sqrt{T_r}) \right]^2$$

Soave 3 constants

$$m_i = m_0 + m_1 \omega_i + m_2 \omega_i^2$$

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

Mixture  $x_i$  eg.

$$\bar{a} = \sum_i \sum_j x_i x_j (a_i a_j)^{0.5} \cdot (1 - k_{ij})$$

$$\bar{b} = \sum_{i=1}^n x_i b_i$$

Liquid mixtures:  $\nu_L$  EOS<sup>2</sup>(SRK/PR) ~ 10-35% high  
wrong!

1981: Peneloux, et al.

$$\nu = \underbrace{\nu^{EOS2}}_c - c$$

$$c = s \cdot b$$

↑  
dimensionless "shift" factor  
(-0.2 → +0.3)

$$\bar{c} = \sum x_i c_i$$

↓  
 $\rho_L \sim 1-3\%$   
( $\rho_V \sim 1-3\%$ )

HQSPS: Allowed  $s_i$  to be input  
(Beware!)

$$\nu = \nu^{EOS2} + c$$

Input " $s_i$ "

$$\left. \begin{array}{l} \text{ECL300} \\ \text{EAP} \end{array} \right\} \text{EOS } \omega / S_i$$

$$\left. \begin{array}{l} \text{Given } x_i \Rightarrow \mu_{Li} \\ \quad \quad \quad \neq \\ y_i \Rightarrow \mu_{Vi} \end{array} \right\} \text{Wrong } K_i$$

P-T FLASH CALCULATION  
(In Each Separator Unit) } Rachford-Rice  
Muskat-McDowell

$$n, z_i \rightarrow \begin{array}{|c|} \hline y_i, n_v \\ \hline x_i, n_L \\ \hline \end{array}$$

$$\begin{aligned} n &= n_v + n_L \\ n_i &= n_{vi} + n_{Li} \\ n z_i &= n_v y_i + n_L x_i \\ \text{Define } \beta &\equiv n_v / n \quad (= F_v) \quad \text{Ch. 3 \& 4} \end{aligned}$$

$(P, T) = \text{Fixed}$

$$\boxed{z_i = \beta y_i + (1 - \beta) x_i} \leftarrow$$

$$z_i \equiv \frac{n_i}{n}$$

$$y_i \equiv \frac{n_{vi}}{n_v}$$

$$x_i \equiv \frac{n_{Li}}{n_L}$$

$$\sum z_i = 1$$

$$\sum y_i = 1$$

$$\sum x_i = 1$$

$$\left. \begin{array}{l} \sum z_i = 1 \\ \sum y_i = 1 \\ \sum x_i = 1 \end{array} \right\} (\sum y_i - \sum x_i) = 0$$

Given:  $z_i$ , Guess set of  $K_i (P, T; z_i)$

Solve:  $\beta, y_i, x_i$

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

$$\Rightarrow \boxed{z_i = \beta y_i + (1-\beta)x_i} \Leftarrow$$

$$\sum y_i - x_i = 0$$

$$z_i = \beta y_i + x_i - \beta x_i$$

$$z_i = \beta K_i x_i + x_i - \beta x_i$$

$$= x_i (\beta K_i - \beta + 1)$$

$$= x_i [\beta(K_i - 1) + 1]$$

$$y_i = K_i x_i$$

$$0 = \sum y_i - x_i$$

$$\sum (K_i - 1) x_i = 0$$

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

$$\left[ \sum \frac{z_i (K_i - 1)}{\beta(K_i - 1) + 1} = 0 \right] = h(\beta) \text{ One unknown } \beta$$

One Eq. (RR)

Muskat-McDowell

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

$$; \quad c_i = 0 \quad \text{for } K_i = 1$$

$$h(\beta) = \sum \frac{z_i}{\beta + c_i} = 0$$

Once  $\beta$  solved:

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

$$y_i = K_i x_i$$

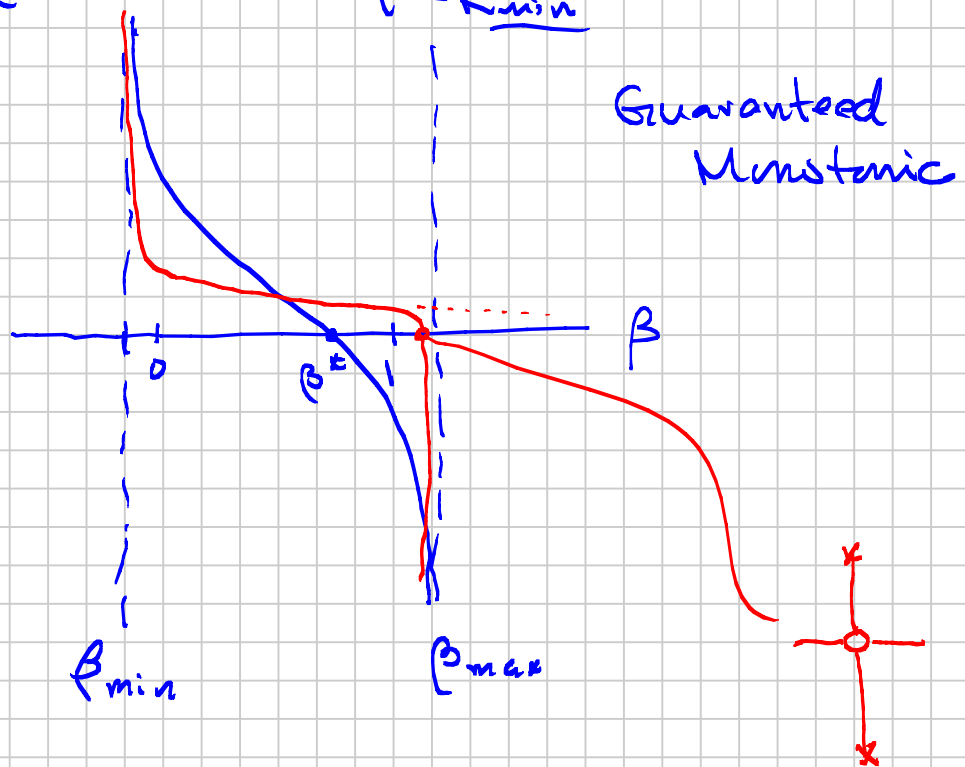


\* Multiple  $\beta$  solutions satisfying the Eq.

\* Only one solution  $\beta^*$  where

ALL  $y_i > 0$   
 $x_i > 0$  } needed to be physical

$$\frac{\beta_{\min}}{1 - K_{\max}} < \beta^* < \frac{\beta_{\max}}{1 - K_{\min}}$$



(g)  $\beta^* < 0$  }  $z_i$  is a single phase

(o)  $\beta^* > 1$

$\beta^* = 0 \in$  :  $z_i = x_i$   
 $z_i$  is a oil at its bubblepoint

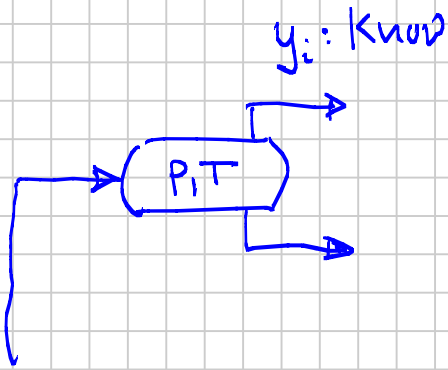
$\beta^* = 1$   
 $z_i$  is a gas at its dewpoint  
 $z_i = y_i$

Got  $y_i \Rightarrow$  EOS  $\left[ \begin{array}{c} \mu_{v,i} \\ = \\ \vdots \\ \mu_{l,i} \end{array} \right] \quad \left| \quad \begin{array}{l} \text{Fugacity } f_i \\ \mu_i \equiv RT \cdot \ln f_i + \text{const} \end{array} \right.$

• Not equal, guess new set  $K_i^{\text{new}} = K_i^{\text{old}} \cdot \left( \frac{f_{v,i}^{\text{old}}}{f_{v,i}} \right)$   
Ch. 4

• Equal, you're done with this unit calculation

App. B Phase Behavior monograph Example



Know:  $y_i, K_i$

Want:  $z_i, x_i, \beta$