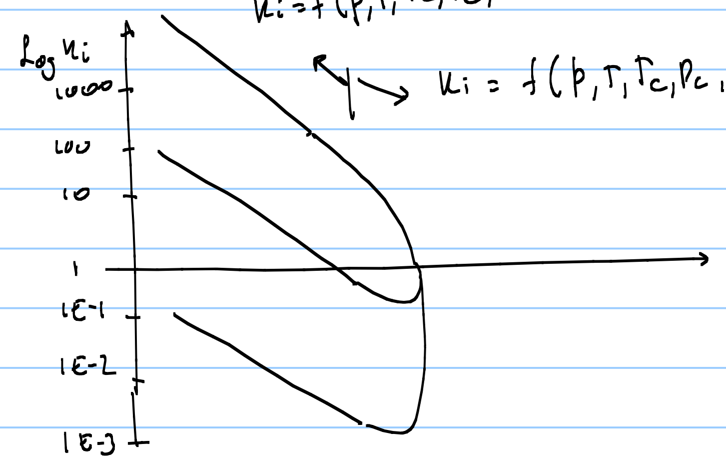
Note Title 15.01.2019

Class 4

$K_i = f(p, T, T_c, P_c, \omega)$

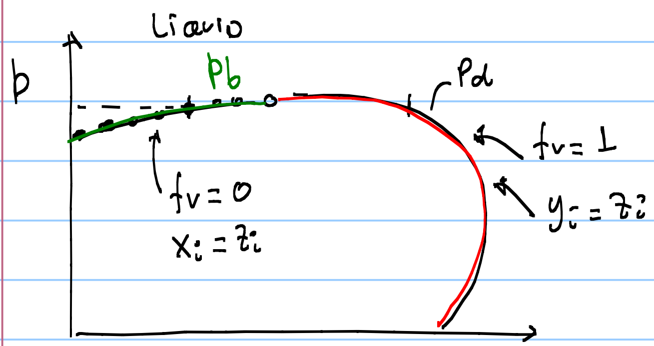


$K_i = f(p, T, T_c, P_c, \omega, P_k)$ → z_i

↳ is representing the composition dependence

K_i from correlation is not very accurate. Is more appropriate for low pressures

Equilibrium calculations can be used to estimate bubble point pressures and dew point pressures



$$h(f_v) = \frac{z_i\,(K_i - 1)}{F_v\,(K_i) - F_v + 1}$$

to find $P_b @ T$, $f_v = 0$, $x_i = z_i$ ⟶ find P such that $h(f_v) = 0$

to find $P_d @ T$, $F_v = 1$, $y_i = z_i$ ⟶ find P such that $h(f_v) = 0$

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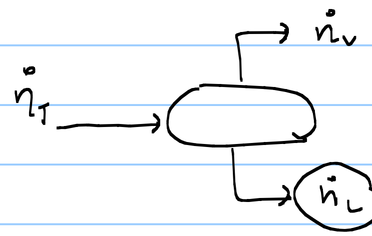
for a mixture, with equilibrium calculations, I am able to estimate

$z_i \to y_i,\ x_i,\ f_v$



$\dot{n}_v = n_T \cdot f_v$

$\dot{n}_L = n_T \cdot (1 - f_v)$

$$\dot{n} \longrightarrow \dot{m} \longrightarrow q\ ?$$

kmol/s kg/s Sm^3/d

$$\dot{n} \cdot \underbrace{MW} = \dot{m}$$

$$q = \frac{\dot{m}}{\rho}\left[\frac{3600 \cdot 24}{1d}\right]$$

ρ @ standard conditions

$$MW_{mix} = \sum_{i=1}^{N} z_i \, MW_i$$

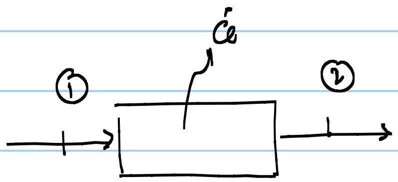
z_i: x_i, y_i

How do we estimate fluid properties? ρ, h, s

analysis of components: heat exchanger, pump, compressor, pipe

μ, k

k: thermal conductivity



$$\dot{Q} = \dot{m}(h_2 - h_1)$$

thermodynamic properties → EOS Equation of state

thermophysical properties

→ correlation

Boyle

Hooke

Charles

Gay-Lussac

Avogadro

ideal gas equation

$$pV = nRT$$

p: Pa, bara

V: m^3

n: mol, kmol

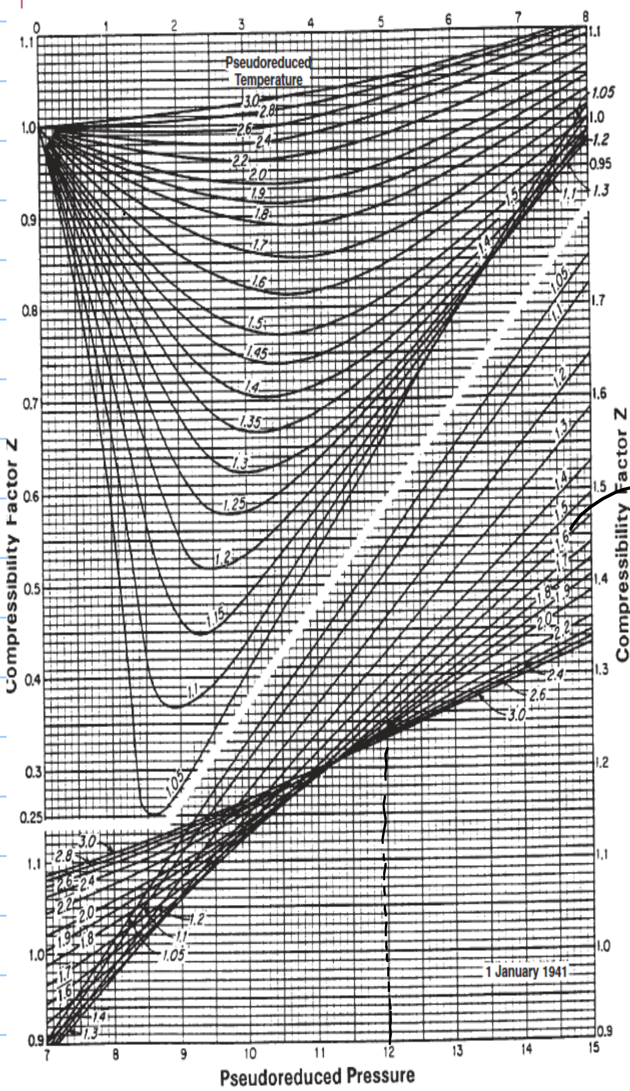
T: K, °R

$R = \frac{pV}{nT} = \left[\frac{Pa}{mol}\,\frac{m^3}{K}\right]$

$pV = nZRT$ $\quad v = \frac{V}{n}$ specific molar volume

Real gas equation $\quad pv = ZRT \rightarrow$ gas deviation factor

gas compressibility factor



$v \longrightarrow \rho$?

$\frac{m^3}{mol} \quad \frac{1}{MW} \quad \left(\frac{m^3}{kg}\right)$

$\rho = \left(\frac{v}{MW}\right)^{-1}$

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

$P_r = \frac{p}{P_c}$

when having a mixture how to estimate P_c T_c?

$\gamma_{gHC} = \frac{\rho_g}{\rho_{air}} = \frac{MW_g}{MW_{air}} = \frac{MW_g}{28.97}$?

$$T_{pcHC} = 169.2 + 349.5\gamma_{gHC} - 74.0\gamma_{gHC}^2$$

nd $p_{pcHC} = 756.8 - 131\gamma_{gHC} - 3.6\gamma_{gHC}^2.$

EOS - Equation of state (PVT calculations)

(Van der Waals)
(1873)

$$p = \underbrace{\frac{RT}{v - b}}_{\text{repulsion term}} - \underbrace{\frac{a}{v^2}}_{\text{attraction term}}$$

$[m^3/mol]$

$$p = \frac{RT}{v}$$

$$p = \frac{RTv^2 - a(v-b)}{(v-b)v^2}$$

$$p(v-b)v^2 - RTv^2 + a(v-b) = 0$$

$pV = ZRT$

$V = \frac{ZRT}{p}$

$$Z^3 - (B + 1)Z^2 + AZ - AB = 0,$$

where $A = a\frac{p}{(RT)^2} = \frac{27}{64}\frac{p_r}{T_r^2}$

and $B = b\frac{p}{RT} = \frac{1}{8}\frac{p_r}{T_r}$. ....

mixing rules are used to find constants for the EOS when there are multi components

Peng Robinson

$$p = \frac{RT}{v - b} - \frac{a}{v(v + b) + b(v - b)}$$

Soave - Redlich Kwong (SRK)

$pV = ZRT$

$V = \frac{ZRT}{p}$ $\qquad V \quad \frac{1}{mol} \left(\frac{1000\ mol}{kmol}\right)$

R	8.31E-06	m^3 MPa/mol-K
T	343.15	[K]
p	5	[Mpa]

Compound	mole frac	Tc	pc	AF (ω)	MW	S	b	m	alpha	a	c	counter	Ai	fugacity
	[-]	[K]	[Mpa]	[-]	kg/kmol	[-]	m^3/mol	[-]	[-]	m^6 MPa/mol^2	m^3/mol		[-]	[Mpa]
C1	0.8196	190.6	4.6	0.0115	16.04	-0.1595	2.68E-05	0.3923	0.7497	1.87E-07	-4.27E-06	1	2.34E-07	3.88E+00
C3	0.1788	369.8	4.3	0.1454	44.09	-0.0863	5.63E-05	0.5932	1.0441	1.06E-06	-4.86E-06	2	5.55E-07	5.99E-01
N-C10	0.0016	617.7	2.1	0.4902	142.29	0.0655	1.91E-04	1.0700	1.6192	9.31E-06	1.25E-05	3	1.61E-06	1.90E-03

BINARY INTERACTION PARAMETERS

	C1	C3	N-C10
C1	0	0.014	0.04361
C3	0.014	0	0
N-C10	0.04361	0	0

PR equation coefficients

amix	2.93E-07	m^6 MPa/mol^2
bmix	3.23E-05	m^3/mol
Amix	1.80E-01	
Bmix	5.66E-02	
a1	-9.43E-01	
a2	5.74E-02	
a3	-0.00682	

Solving PR cubic equation

			if M<0 then			**If M>0 then**	
Q	0.080		**teta**	NA	**fugacity**	**S'**	0.334
R	-0.025		**z1**	NA	NA	**T'**	0.239
M	1.42E-04		**z2**	NA	NA	**z**	8.87E-01
			z3	NA	NA		
MW	21.3	kg/kmol					
z	8.87E-01						
v	5.06E-01	m^3/kmol					
v_corrected	5.11E-01	m^3/kmol					
v	2.40E-02	m^3/kg					
den	41.64	kg/m^3					

with EOS one can calculate other properties, h, u, s

- definition of property $h = u + p \cdot v$
- first law $dU = dQ - dW$
- fundamental relationships between derivatives of properties

$$d\underline{U} = C_V dT + \left[T\left(\frac{\partial P}{\partial T}\right)_{\underline{V}} - P \right] d\underline{V}$$

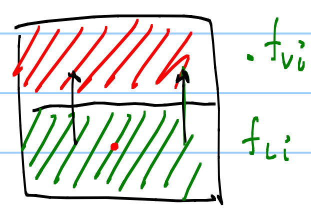
$$d\underline{U} = C_v dT + \left[T\underline{\left(\frac{\partial p}{\partial T}\right)_V} - p \right] d\bar{V}$$

$$\frac{\partial p}{\partial T} = \frac{RT}{v-b} - \frac{a}{v(v+b)+b(v-b)}$$

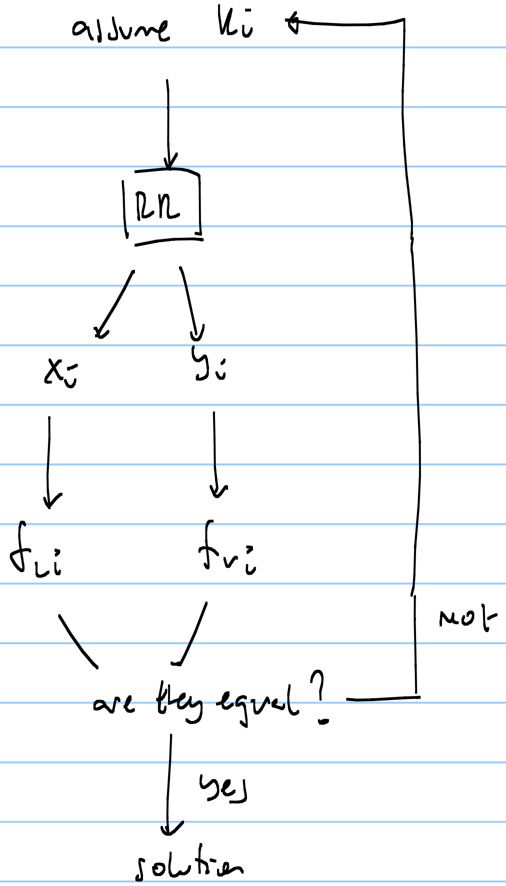
one can calculate a property called chemical energy f_i

$$\ln \frac{f_i}{y_i p} = \ln \phi_i = \frac{B_i}{B}(Z-1) - \ln(Z-B) + \frac{A}{2\sqrt{2}B}\left(\frac{B_i}{B} - \frac{2}{A}\sum_{j=1}^{N} y_j A_{ij}\right) \ln\left[\frac{Z+\left(1+\sqrt{2}\right)B}{Z-\left(1-\sqrt{2}\right)B}\right]$$

in a mixture $\boxed{f_{Li} = f_{vi}}$



I can use EOS to find K_i



VLE calculations