COMPOSITIONS

Note Title 1/30/2017

Compositional Information – Summary

* Molar Amounts

n_i $\quad n_{gi}$ $\quad n_{oi}$ — mol (= gmole) | kmol = kg-mole, lb-mole

z_i $\quad y_i$ $\quad x_i$ $\quad (u_i)$ — Mole Fractions $\Sigma = 1$

i: $z_i \equiv \frac{n_i}{n}$ $\quad y_i = \frac{n_{ig}}{n_g}$ $\quad x_i = \frac{n_{io}}{n_o}$ | e.g. $n_g = n_o$, y_{c_1} vs x_{c_1}

* Molecular Mass (Weight)

$M \equiv \frac{m}{n}$ relates mass to mole (with consistent mass units)

$M_{c_1} = 16.04 \frac{g}{mol}$, $16.04 \frac{kg}{kmol}$, $16.04 \frac{kg}{kgmole}$

* Mass Amounts (Measured in lab)

m_i $\quad m_{gi}$ $\quad m_{oi}$ — mass

$w_i = \frac{m_i}{m}$ $\quad w_{gi} =$ $\quad w_{oi}$ — mass fractions (weight), $\Sigma w_i = 1$

$y_{c_1} \cdot n_g = (n_{c_1})_g > (n_{c_1})_o = x_{c_1} \cdot n_o$

$y_{c_1} > x_{c_1}$ $\qquad \underline{\underline{K_i}} \equiv \left(\frac{y_i}{x_i}\right) > 1$ for C_1

Any value of n_g, n_o

632 lb-moles of a gas

How many g-moles?

632 lb-moles $\cdot\ 0.453 \cdot 10^3 \frac{\text{g-moles}}{\text{lb-moles}} = \underline{286 \cdot 10^3}$ g-mole, mol

$2.204 \frac{lb}{kg} \times \frac{kg}{1000\,g}$

$2.204 \cdot 10^{-3} \frac{lb}{g}$

$0.453 \cdot 10^3 \frac{g}{lb}$

$0.453 \cdot 10^3 \cdot \frac{\text{g-mole}}{\text{lb-mole}}$

TABLE 2.1—COMPOSITION AND PROPERTIES OF SEVERAL RESERVOIR FLUIDS

			Composition (mol%)			
Component	Dry Gas	Wet Gas	Gas Condensate	Near-Critical Oil	Volatile Oil	Black Oil
CO_2	0.10	1.41	2.37	1.30	0.93	0.02
N_2	2.07	0.25	0.31	0.56	0.21	0.34
C_1	86.12	92.46	73.19	69.44	58.77	34.62
C_2	5.91	3.18	7.80	7.88	7.57	4.11
C_3	3.58	1.01	3.55	4.26	4.09	1.01
i-C_4	1.72	0.28	0.71	0.89	0.91	0.76
n-C_4		0.24	1.45	2.14	2.09	0.49
i-C_5	0.50	0.13	0.64	0.90	0.77	0.43
n-C_5		0.08	0.68	1.13	1.15	0.21
$C_{6(s)}$		0.14	1.09	1.46	1.75	1.61
C_{7+}		0.82	8.21	10.04	21.76	56.40
			Properties			
$M_{C_{7+}}$		130	184	219	228	274
$\gamma_{C_{7+}}$		0.763	0.816	0.839	0.858	0.920
K_{wC_7}		12.00	11.95	11.98	11.83	11.47
GOR, scf/STB	∞	105,000	5,450	3,650	1,490	300
OGR, STB/MMscf	0	10	180	275		
γ_{API}		57	49	45	38	24
γ_g		0.61	0.70	0.71	0.70	0.63
p_{sat}, psia		3,430	6.560	7,015	5,420	2,810
B_{sat}, ft^3/scf or bbl/STB		0.0051	0.0039	2.78	1.73	1.16
ρ_{sat}, lbm/ft^3		9.61	26.7	30.7	38.2	51.4

C_{6+} C_{n+}

K_w = Watson (UOP) Characterization Factor

$$\equiv \frac{T_b(°R)^{1/3}}{\gamma_L} \quad \text{Liquid @ STC}$$

[8   9   [10   11   12] 12.5]   13]

"Aromatic"-ish 10.5   SCN   12.2 — C_{7+} "Paraffic"-ish

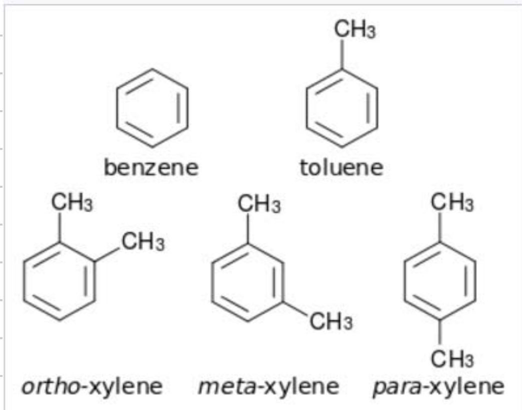
(SCN)
Single Carbon Number mixture

"C_7" all isomers boiling at 1 atm (T_b)

$$T_{b_{n\text{-}C_6}} < T_b \le T_{b_{n\text{-}C_7}} \qquad >6 \quad <100$$

$(T_b)_{SCN,C_7}$

BTEX
- Benzene C_6H_6
- Tolnene C_7
- Ethylbenzene
- Xylene(s)



Structural diagrams of the BTX hydrocarbons.

Further description:- Benzene, toluene, ethylbenzene, and xylene

Glossary Entry

BTEX is an acronym for benzene, toluene, ethylbenzene, and xylene. This group of volatile organic compounds (VOCs) is found in petroleum hydrocarbons, such as gasoline, and other common environmental contaminants.

The monoaromatic hydrocarbons, abbreviated BTEX, which stands for benzene, toluene, ethylbenzene, trimethylbenzenes and the three xylene isomers, are aromatic hydrocarbons containing one unsubstituted or methyl-substituted benzene ring, See Figure 1.

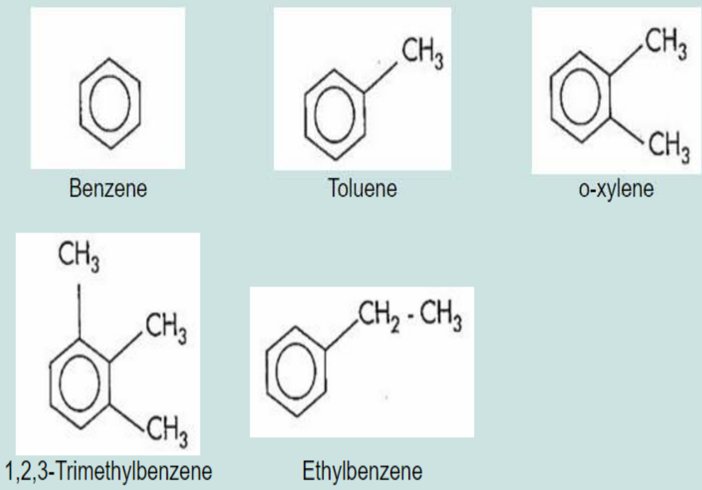


Figure 1. Structure formula for the BTEX.

BTEX have in recent years attracted much attention, since they constitute one of the most common and serious threats to groundwater reservoirs and indoor climate deriving from contaminated sites. This is mainly due to the potential effects of benzene, which is considered a strong carcinogen, and which is highly mobile in the soil and groundwater environment, which is also the case for the other BTEX.

Molar Mass

Ideal Volumes ($V_{\bar{o}i}, V_{\bar{g}i}$)

valid at STC (standard conditions) for HCs

* $V_{\bar{o}} \cong \sum V_{\bar{o}i}$; $V_{\bar{o}i} \equiv \frac{m_i}{\rho_{\bar{o}i}}$; $\rho_{\bar{o}i}$ = component i liquid density at STC

$$V_{\bar{g}} \cong \sum V_{\bar{g}i} \; ; \quad V_{\bar{g}i} \equiv \underbrace{\left(\frac{RT_{sc}}{p_{sc}}\right)}_{23.68\ Sm^3/kg\text{-}mole} n_i = \left(\frac{RT_{sc}}{M_i p_{sc}}\right) m_i$$

Averaging Properties

Average surface oil densities
(STO, STC, SO, $\bar{o}$ | C_{7+}, C_{n+})
all liquids at STC

$$\frac{m_{\bar{o}}}{V_{\bar{o}}} = \rho_{\bar{o}} \cong \frac{\sum m_i}{\sum V_{\bar{o}i}} = \frac{\sum m_i}{\sum \frac{m_i}{\rho_{\bar{o}i}}} = \frac{\sum w_i}{\sum \frac{w_i}{\rho_{\bar{o}i}}}$$

Ideal Volume Mixing

e.g. Calculation C_{6+} ⟨ M_{6+}, ρ_{6+} ⟩ to convert C_{6+} mol-%'s to GOR

C_{7+} MW & ρ always reported by the lab

C_6 <u>Table 5.2</u> as an average

GAS COND. Reservoir Fluid

$M_{C_6} = 84$ $\qquad M_{7+} = 184$ $\qquad z_{C_6} = 1.09$

$\gamma_{C_6} = 0.69$ $\qquad \gamma_{7+} = 0.816$ $\qquad z_{7+} = 8.21$

$$M_{6+} = \frac{\overset{m_{C_6}}{1.09(84)} + \overset{m_{C_{7+}}}{8.21(184)}}{(\underset{n_{C_6}}{1.09} + \underset{n_{C_{7+}}}{8.21})} = \_\_\_\_$$

z_{6+} ↓ GOR

$$\gamma_{6+} = \frac{1.09(84) + 8.21(184)}{\frac{1.09(84)}{0.69} + \frac{8.21(184)}{0.816}} = \_\_\_\_$$

TABLE 5.2—SINGLE CARBON NUMBER PROPERTIES FOR HEPTANES-PLUS (after Katz and Firoozabadi[6])

	Katz-Firoozabadi Generalized Properties								Lee-Kesler[12]/Kesler-Lee[13] Correlations			Riazi[14]	Defined
	T_b Interval*		Average T_b										
Fraction Number	Lower (°F)	Upper (°F)	(°F)	(°R)	γ*	M	Defined K_w		T_c (°R)	p_c (psia)	ω	V_c (ft³/lbm mol)	Z_c
6	97.7	156.7	147.0	606.7	0.690	84	12.27		914	476	0.271	5.6	0.273
7	156.7	210.0	197.4	657.1	0.727	96	11.96		976	457	0.310	6.2	0.272
8	210.0	259.0	242.1	701.7	0.749	107	11.86		1,027	428	0.349	6.9	0.269
9	259.0	304.3	288.0	747.6	0.768	121	11.82		1,077	397	0.392	7.7	0.266
10	304.3	346.3	330.4	790.1	0.782	134	11.82		1,120	367	0.437	8.6	0.262
11	346.3	385.5	369.0	828.6	0.793	147	11.84		1,158	341	0.479	9.4	0.257
12	385.5	422.2	406.9	866.6	0.804	161	11.86		1,195	318	0.523	10.2	0.253

$$GOR = f\left(z_{n+}, \left(\frac{M}{\rho}\right)_{n+}\right)$$

How does the lab measure compositions? (of reservoir fluids)

GAS CHROMATOGRAPHY

(1) Separator Sample → GAS SAMPLE ← ① Flashed Gas (to 1 atm)

① "FLASHED" (to 1 atm) OIL SAMPLE

Austad et al.

BHS

1 phase @ T_R, $P_R > P_s$

Flash to 1 atm

① Flashed Gas → GC

① Flashed Oil → GC

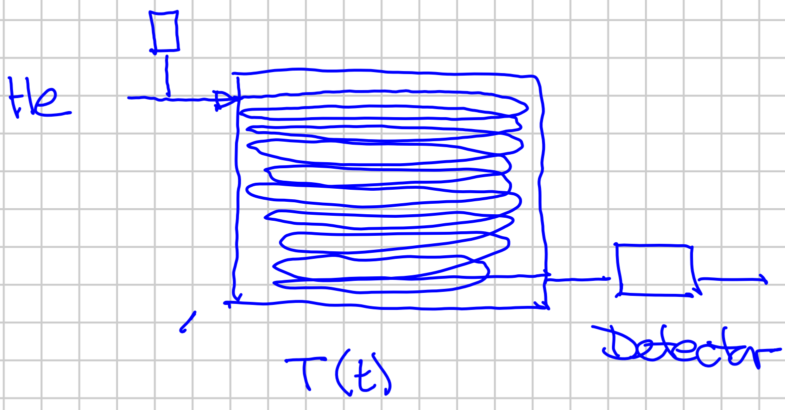
SEP (Separator Samples)

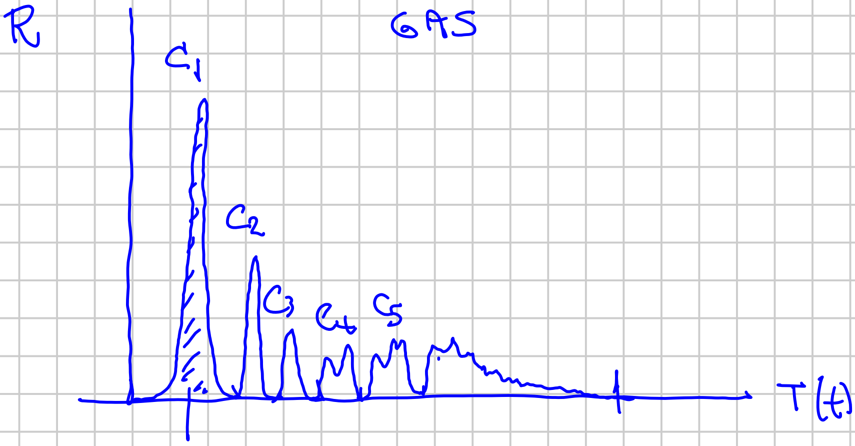
(2) 20 L sep. Gas

~1 L Sep Oil

Flash to 1 atm

① Flashed Gas + Flashed Oil





$A_i \propto m_i$

$$w_i = \frac{A_i}{\{\sum A_j\}_{seen}} \quad \checkmark$$

M_i known ✓

$$\Rightarrow y_i = \frac{w_i / M_i}{\sum w_j / M_j} \quad \checkmark$$

FLASHED OIL