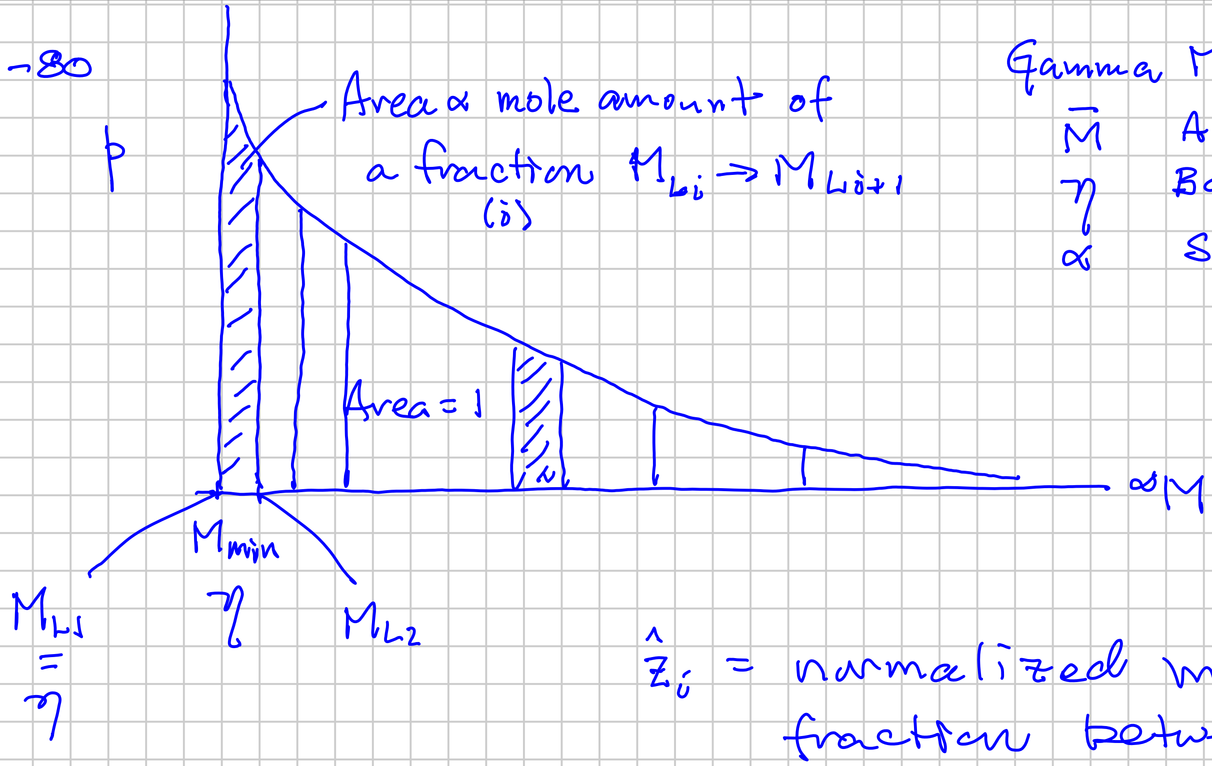
Molar Distribution of C_{n+} in Petroleum Mixtures

Note Title 2/25/2016

1979-80



Gamma Model

$\bar{M}$ AVERAGE

η BOUND

α SHAPE

$\hat{z}_i$ = normalized mole fraction between M_{Li} and M_{Li+1} in a C_{n+} mixture

$\Delta M_{Li} = 14$ SCN

n : choice of η

$$\hat{z}_i = \int_{M_{Li}}^{M_{Li+1}} p(M)\, dM$$

Actual molar amount in the reservoir fluid

$z_{n+} = 20$ mol-%

$z_{i=7} = \hat{z}_7 \cdot z_{n+}$

$$\bar{M}_i = \left(\int_{M_{Li}}^{M_{Li+1}} p \cdot M \, dM \right) \Big/ \hat{z}_i$$

$$\hat{z}_i = \int_{\eta}^{\infty} p \, dM = 1 \qquad M_{n+} = \frac{\int_{\eta}^{\infty} p \cdot M \cdot dM}{\int_{\eta}^{\infty} p \, dM}$$

Solve Gamma model generically

$$x = \frac{M-\eta}{\beta} \quad \Big| \quad \beta \equiv \frac{\bar{M}_{n+} - \eta}{\alpha}$$

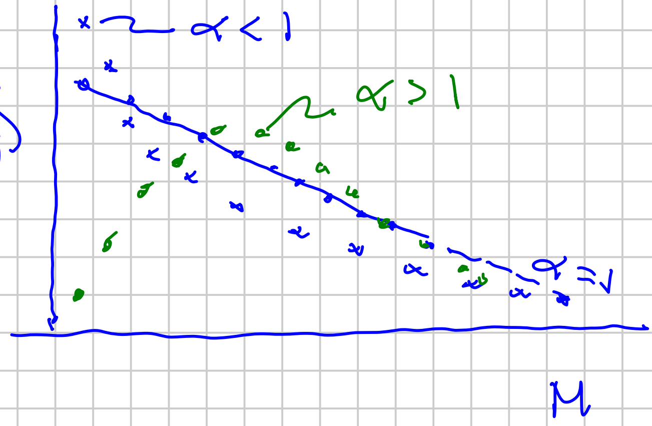
Shape α

$\alpha = 1$: exponential (log)

$\alpha < 1$: accelerated exponential

$\alpha > 1$: skewed

$\alpha \approx \infty$: log-normal



Summarize Gamma Distribution Model

1. Select what mixture to model C_{n+}
2. $\bar{M}_{n+}$
3. η : $\Leftrightarrow$ "n" $\qquad \eta \sim 14 \cdot n - \Delta$ ~ 7-ish
4. α : Shape
5. M_{Li} mol wt. bounds to discretize and get something useful z_i $\bar{M}_i$
   - Choice of LMW bounds ~ arbitrary or based the measured data z_i & $\bar{M}_i$

Commercial PVT Labs Compositional Data:

Measure mass amounts weight

< 1980	:	C_{7+}		
90s	:	C_{10+}	C_{12+}	C_{15+}
2000-09	:	C_{21+}	C_{30+}	
> 2000	:	C_{30+}	C_{36+}	

Today's Standard

Gamma model of C_{15+}

Molar Distribution $\Downarrow$ Mass Distribution $z_i \sim M_i$ $\underbrace{z_i(M_i)}_{w_i}$

$$w_i = \frac{z_i \bar{M}_i}{\sum_{j=n}^{N+} z_i \bar{M}_i}$$

Alternatives :

Discrete SCN model – exponential (PVTsim)

$$\hat{z}_i = \hat{z}_n \cdot \exp[A(i-n)]$$

$i = n$ (e.g. C_{7+} $n=7$) $\hat{z}_7 = \tilde{z}_7$

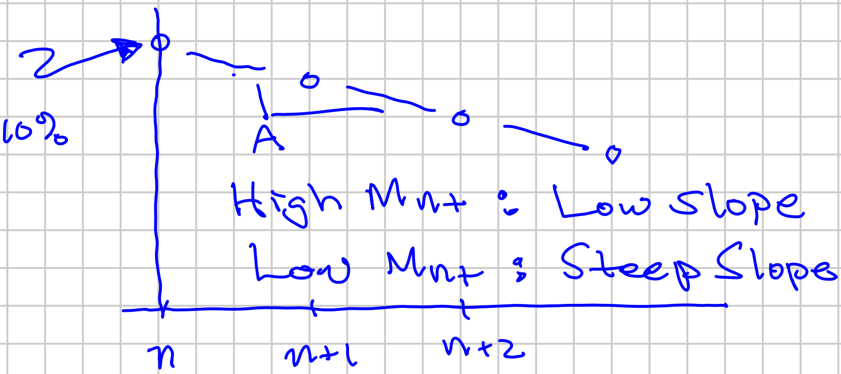
$$M_i = 14i + h$$

specified (PVTsim $h=-4$)

A : slope on a plot $\log z_i$ vs SCN

$\hat{z}_n$ = e.g. 0.1 = 10%

% of the C_{n+} that is found in the first SCN



$$\left(\frac{z_i - z_{i+1}}{z_i}\right) = 10\% = \hat{z}_n$$

$z_n = 0.1$ $z_{n+1} = 0.1 - 0.1(0.1) =$

$A\ (M_{n+})$:

$$\hat{z}_i = \hat{z}_{C_n} \exp A[(i - n)], \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (5.7)$$

where i = carbon number, $\hat{z}_{C_n}$ = mole fraction of C_n, and A = constant indicating the slope on a plot of $\ln \hat{z}_i$ vs. i. The constants $\hat{z}_{C_n}$ and A can be determined explicitly. With the general expression

$$M_i = 14i + h \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (5.8)$$

for molecular weight of C_i and the assumption that the distribution is infinite, constants z_{C_n} and A are given by

$$\hat{z}_{C_n} = \frac{14}{\boxed{M_{C_{n+}}} - 14(n-1) - \boxed{h}} \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (5.9)$$

and $A = \ln\left(1 - \hat{z}_{C_n}\right) \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (5.10)$

slope

so that $\sum_{i=n}^{\infty} \hat{z}_i = 1 \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (5.11)$

Apply the Gamma Distribution Model

- Fit the reported molar distributions for HCH oil & gas samples.

Assume Gamma Model

$\bar{M}_{7+} = 199$

$\eta = 90$

$\alpha > 1 \quad (1.5)$

Modify these to minimize the mismatch of Gamma model z_i & $\bar{M}_i$ vs Lab data

Phazecomp (Excel) : (1) Guess/estimate M_{Li}

(1)

(2) Let the program calculate M_{Li+1} to satisfy reported data for each i z_i & M_i

(2) b

a
$$\frac{\int_{M_{Li}}^{M_{Li+1}} p \cdot M \, dM}{\int_{M_{Li}}^{M_{Li+1}} p \, dM} = \text{Lab } \bar{M}_i$$

b
$$\int_{M_{Li}}^{M_{Li+1}} p \, dM = \text{Lab } \frac{z_i}{z_{7+}} \qquad \frac{w_i}{w_{7+}}$$

$$\text{Mismatch} \quad \min. \sum_{i=1}^{N-1 \; :34} \left[\frac{(\bar{M}_i)_G - (\bar{M}_i)_{Lab}}{\bar{M}_{7+}} \right]^2$$

by changing

$(\vec{M}, \eta, \alpha)$

Method ① M_{Li} are specified

(a) $\Delta M_{Li} = 14$

(b) $M_{Li} = \frac{1}{2}(\vec{M}_i + \vec{M}_{i+1})$

PhZ (c) $M_{Li} = f(i, \text{P-A})$ unpublished

⋮

(I) Mismatch min. $\sum_{i=7}^{N-1 = 34} \left[\frac{(\vec{M}_i)_G - (\vec{M}_i)_{Lab}}{\vec{M}_{7+}} \right]^2$

(II) Mismatch $\sum_{i=7}^{34} \left[(\hat{z}_i)_G - (\hat{z}_i)_{Lab} \right]^2$

$(w_i)_G - (w_i)_{Lab}$