[Numerical on $\overline{M_n}$, $\overline{M_w}$, PDI]

1) In a polymer, there are 100 molecules of molecular weight 100, 200 molecules of molecular weight 1000, and 300 molecules of molecular weight 10,000.

Find $\overline{M_n}$, $\overline{M_w}$, PDI.

Solution:

(i) $$\overline{M_n} = \frac{\Sigma N_i M_i}{\Sigma N_i} = \frac{N_1 M_1 + N_2 M_2 + N_3 M_3}{N_1 + N_2 + N_3}$$

$$\overline{M_n} = \frac{(100 \times 100) + (200 \times 1000) + (300 \times 10000)}{100 + 200 + 300}$$

$$\left[\overline{M_n} = \frac{3.21 \times 10^6}{600} = 5.35 \times 10^3\right]$$

(ii) $$\overline{M_w} = \frac{\Sigma N_i M_i^2}{\Sigma N_i M_i} = \frac{100 \times (100)^2 + 200 \times (1000)^2 + 300 \times (10000)^2}{(100 \times 100) + (200 \times 1000) + (300 \times 10{,}000)}$$

$$\left[\overline{M_w} = 9.4 \times 10^3\right]$$

(iii) $$PDI = \frac{\overline{M_w}}{\overline{M_n}} = \frac{9.4 \times 10^3}{5.35 \times 10^3}$$

$$\left[PDI = 1.757\right]$$

2) A polymer mixture prepared by mixing 3 polymers A, B & C having $\overline{M_n}$, $\overline{M_w}$ & weights in mixture as given below:

Polymer	$\overline{M_n}$	$\overline{M_w}$	wt. in ~~mixture~~ mixture (gm)
A	1.2×10^5	4.5×10^5	200
B	5.6×10^5	8.9×10^5	200
C	10×10^5	10×10^5	100

Find $\overline{M_n}$ & $\overline{M_w}$ of mixture.

<u>Solution</u>:

$$\left(\overline{M_n}\right)_A = \frac{\Sigma W_A}{\Sigma N_A}$$

Hence, $\Sigma N_A = \dfrac{\Sigma W_A}{\left(\overline{M_n}\right)_A}$

$$\left(\overline{M_n}\right)_{mix.} = \frac{(\Sigma W)_{mix}}{(\Sigma N_i)_{mix}} = \frac{W_A + W_B + W_C}{N_A + N_B + N_C}$$

$$= \frac{W_A + W_B + W_C}{\frac{W_A}{\left(\overline{M_n}\right)_A} + \frac{W_B}{\left(\overline{M_n}\right)_B} + \frac{W_C}{\left(\overline{M_n}\right)_C}}$$

$$= \frac{200 + 200 + 100}{\frac{100}{1.2\times10^5} + \frac{200}{5.6\times10^5} + \frac{100}{10\times10^5}}$$

$$\boxed{\left(\overline{M_n}\right)_{mix} = 2.35\times10^5}$$

$$\overline{M_w} = \frac{\Sigma N_i M_i^2}{\Sigma N_i M_i} = \frac{\Sigma W_i N_i}{\Sigma W_i}$$

$$(\overline{M_w})_A = \frac{\Sigma W_A N_A}{\Sigma W_A}$$

$$\therefore \Sigma W_A N_A = (\overline{M_w})_A \cdot \Sigma W_A$$

$$\therefore (\overline{M_w})_{mix} = \frac{\Sigma(W_A N_A) + \Sigma(W_B N_B) + \Sigma(W_C N_C)}{\Sigma(W_A + W_B + W_C)}$$

But,

$$= \frac{(\overline{M_w})_A \Sigma W_A + (\overline{M_w})_B \Sigma W_B + (\overline{M_w})_C \Sigma W_C}{200 + 200 + 100}$$

$$= \frac{(4.5\times10^5 \times 200) + (8.9\times10^5 \times 200) + (10\times10^5 \times 100)}{500}$$

$$\boxed{(\overline{M_w})_{mix} = 7.36 \times 10^5}$$

1) Calculate $\overline{M_n}$ & $\overline{M_w}$ of polypropylene polymer with the following composition.

a) $\left[CH_2-\overset{CH_3}{\overset{|}{CH}}\right]_{400}$ is 25 %

b) $\left[CH_2-\overset{CH_3}{\overset{|}{CH}}\right]_{800}$ is 35 %

c) $\left[CH_2-\overset{CH_3}{\overset{|}{CH}}\right]_{600}$ is 40 %

[Given, Atomic mass of C=12 , H=1]

<u>Solution</u>: Molecular mass of (a) $=[(12\times3)+(6\times1)]\times400$

$M_1 = 16800$

Molecular mass of (b) $=[(12\times3)+(6\times1)]\times800$

$M_2 = 33600$

Molecular mass of (c) $=[(12\times3)+(6\times1)]\times600$

$M_3 = 25200$

$n_1 = 25, \quad n_2 = 35, \quad n_3 = 40.$

Thus $\overline{M_n} = \dfrac{n_1M_1 + n_2M_2 + n_3M_3}{n_1+n_2+n_3}$

$\overline{M_n} = \dfrac{(25\times16800) + (35\times33600) + (40\times25200)}{100}$

$\overline{M_n} = 26040$

And, $\overline{M_w} = \dfrac{n_1M_1^2 + n_2M_2^2 + n_3M_3^2}{n_1M_1 + n_2M_2 + n_3M_3}$

$\overline{M_w} = \dfrac{7.1966\times10^{10}}{2604000} = \underline{27637}$