

How to calculate M_n , M_w and M_z

from raw molecular weight data for resin PBR0

Calculations

From the presentation:
"Moments of Distribution"

1

$$(1) \quad M_n = \frac{\sum N_i M_i}{\sum N_i}$$

$$(2) \quad M_w = \frac{\sum N_i M_i^2}{\sum N_i M_i}$$

$$(3) \quad M_w = \frac{\sum N_i M_i^3}{\sum N_i M_i^2}$$

3

This is the data in the excel file
6) Case Fiber Spinning MWD PB Resins

4

NOTE:
I added a column so, you can
see that there are 115 chains
of different sizes

2

Where:

N_i is the amount of
molecules of size M_i

and

M_i is the molecular weight
of the i th chain and is
represented by M_{wi}

The number of i chains is
the one given to you on a
list

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i <i>chain</i>	M_{wi}	Weight fraction (X_i) of each M_i for the PBR0 resin
1	4956437	0.04
2	4630417	0.04
3	4325840	0.05
4	4041299	0.06
5	3775473	0.07
6	3527133	0.08
7	3295128	0.10
8	3078383	0.12
9	2875896	0.14
10	2686727	0.16

The number of moles is equal to:

$$N_i = X_i (\text{grs}) / M_{wi} (\text{grs/mol}) = \text{moles}$$

$$(1) \quad M_n = \frac{\sum \frac{X_i}{M_i} M_i}{\sum \frac{X_i}{M_i}} = \frac{\sum X_i}{\sum \frac{X_i}{M_i}}$$

Calculations for Mw and Mz:

$$M_w = \frac{\sum \frac{X_i}{M_i} M_i^2}{\sum \frac{X_i}{M_i} M_i} = \frac{\sum X_i M_i}{\sum X_i} \quad (2)$$

$$M_z = \frac{\sum \frac{X_i}{M_i} M_i^3}{\sum \frac{X_i}{M_i} M_i^2} = \frac{\sum X_i M_i^2}{\sum X_i M_i} \quad (3)$$

You have X_i and M_i for each resin, so you can now calculate the average numbers

Steps

1. Observe that Column B gives you the molecular weight for each of the 116 chains as reported by Gel Permeation Chromatography (GPC) measurements.
2. Observe that column C gives you the grams of each chain and the sum should be 100 grs (if not normalize the data so the sum is 100)
3. Go to cell C118 and make sure that the summation of the weights gives you 100
4. Do the calculation of M_n on cell C119 using equation 1 from slide 2
5. Do the calculation of M_w on cell C120 using equation 2 from slide 3
6. Do the calculation of M_z on cell C121 using equation 3 from slide 3

Hint (use the sumproduct function)