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**Viscoelasticity Maxwell Model & Molecular Weight Distribution**

# Viscoelasticity Maxwell Model

INSTRUCTIONS

Fit the relaxation modulus G(t) of the two materials (PBR8, HDPE) using as many Maxwell elements as needed. Plot each Maxwell element in the same plot of G(t) vs. time to show that by adding them up you can fit the experimental curve

AVAILABLE DATA

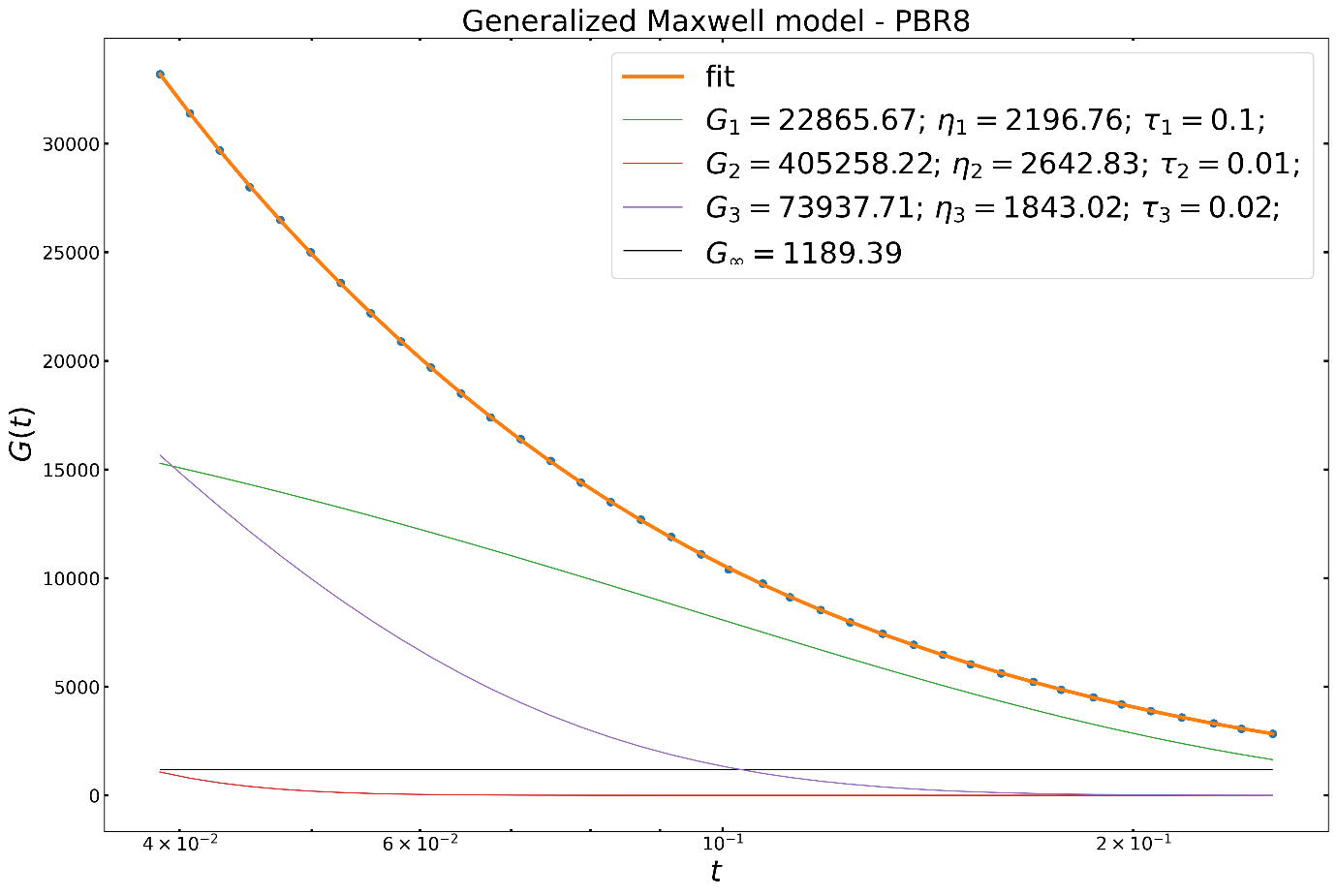
* Relaxation modulus G(t) of two materials (PBR8, HDPE)

ASSUMPTIONS

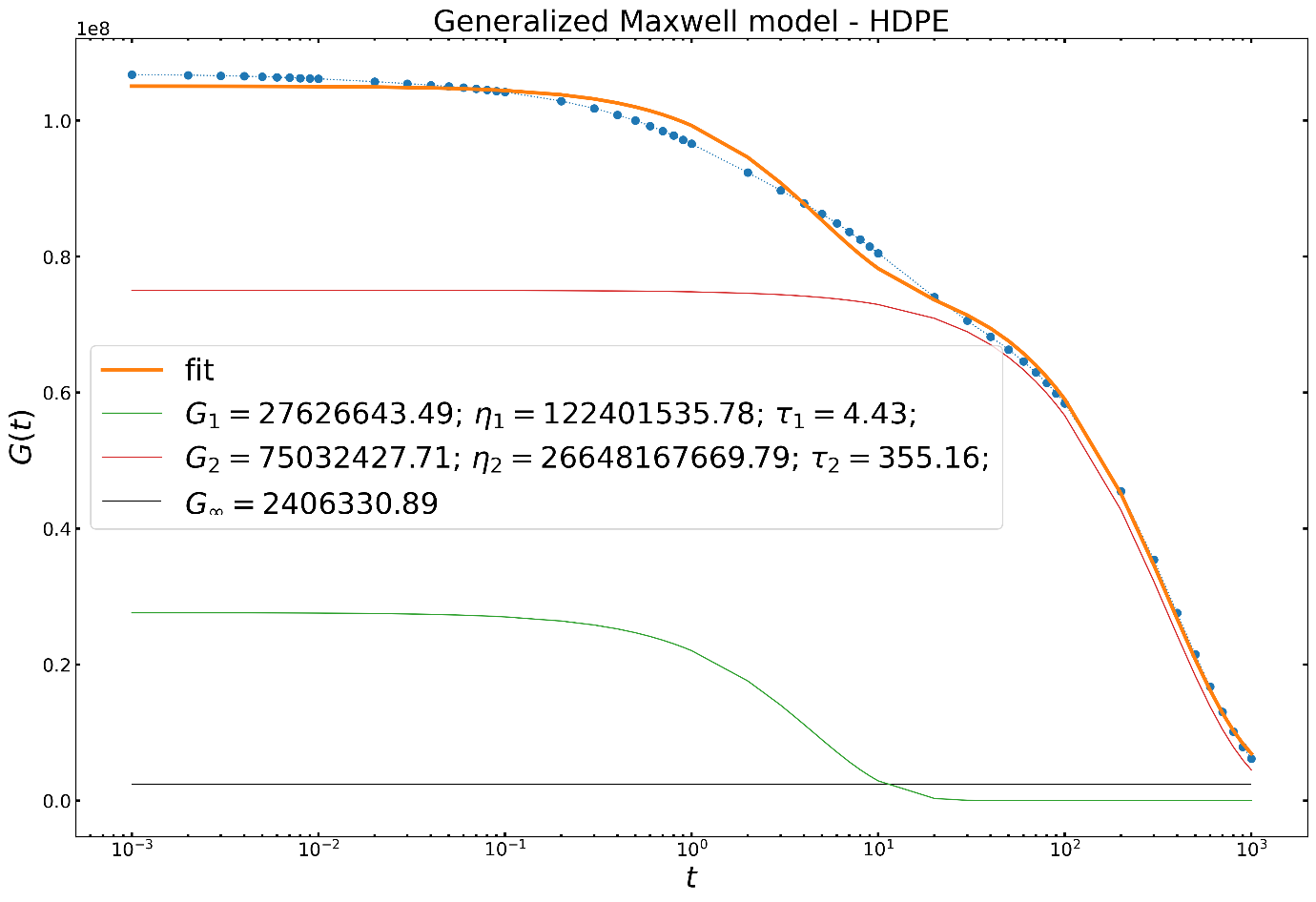
ALGORITHM

* Define the Generalized Maxwell model
* Fit the model to the given G versus t data
* Save the fitting parameters for each Maxwell element
* Plot the data and the model using the fitting parameters

SOLUTION



(Juan)



* A higher n value may achieve a higher fitting accuracy, but also involves more complexity.

REFERENCES

D. Roylance, Engineering Viscoelasticity, in: D. of M.S. and Engineering (Ed.), Massachusetts Institute of Technology, Cambridge, MA, 2001: pp. 1–38. http://web.mit.edu/course/3/3.11/www/modules/visco.pdf.

# Molecular Weight Distribution

INSTRUCTIONS

Given the data listed below: a) calculate the Mn, Mw, Mz and PDI for the PAR0, PAR5, PBR0 and PBR8 resins. Report the results in table; b) plots for the molecular weight distribution of the pairs “PAR0 & PAR5” and “PBR0 & PBR8”; and c) Report the observations of the calculated average molecular weights and MWDs.

AVAILABLE DATA

* Molecular weight of the ith chain (Mwi) of several samples (PAR0, PAR5, PBR0, PBR8)
* Weight fraction (Xi) of each Mwi for several samples (PAR0, PAR5, PBR0, PBR8)

ASSUMPTIONS

1. Je(t) and Jr(t) are the same thing.
2. In graph (2) the X axis should be time, and not shear rate.
3. In graph (4) the Y axis should be Jr(t), and not N1.

ALGORITHM

1. Ensure the weight fraction Xi is normalized. (The sum should give 100 grs)
2. Compute the number of molecules of size Mi
3. Compute the number average molecular weight Mn
4. Compute the weight average molecular weight Mw
5. Compute the higher average molecular weight Mz
6. Compute the polydispersity index PDI
7. Build the requested table containing the previous calculations
8. Plot the MWD in pairs for each sample series

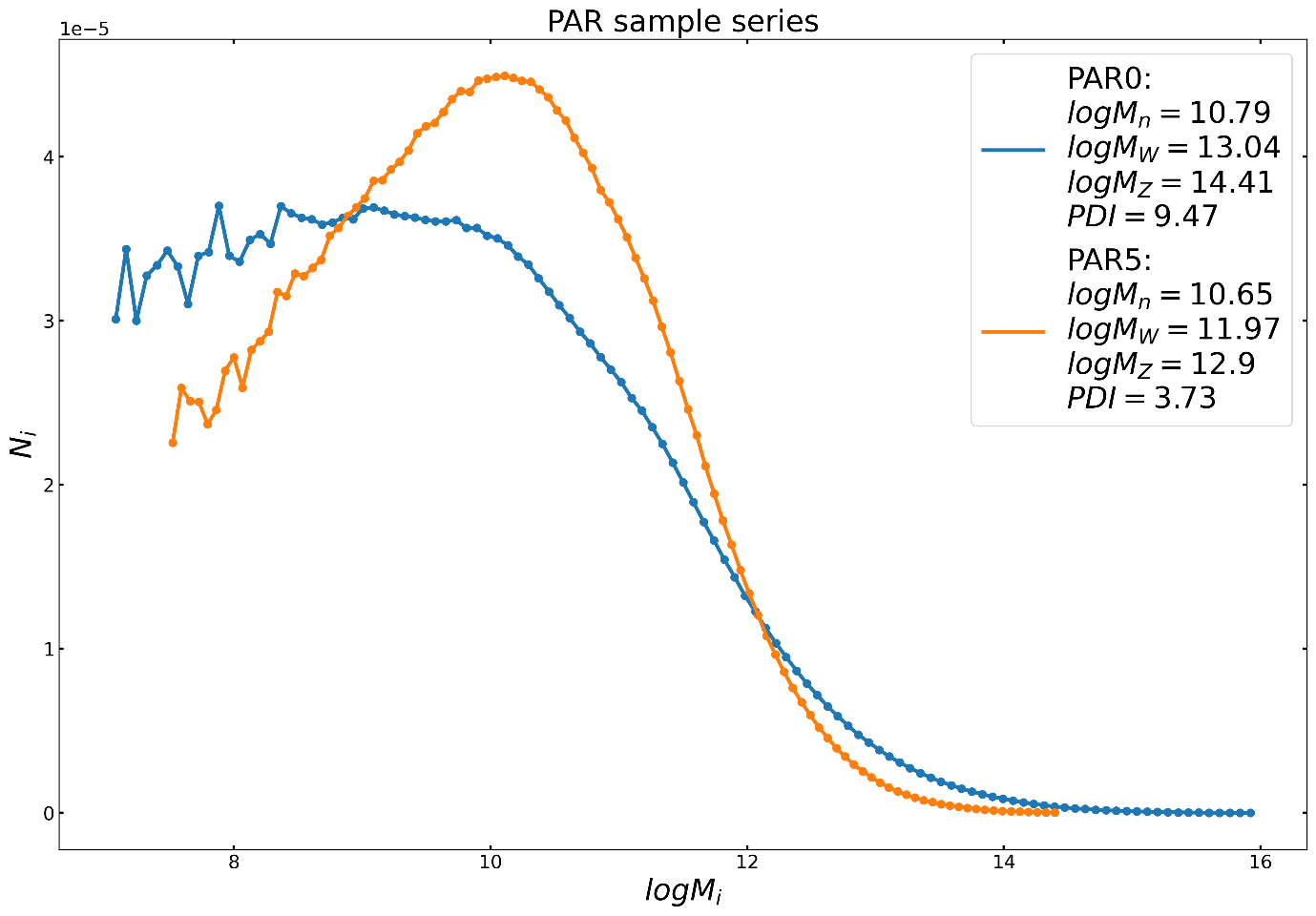
SOLUTION

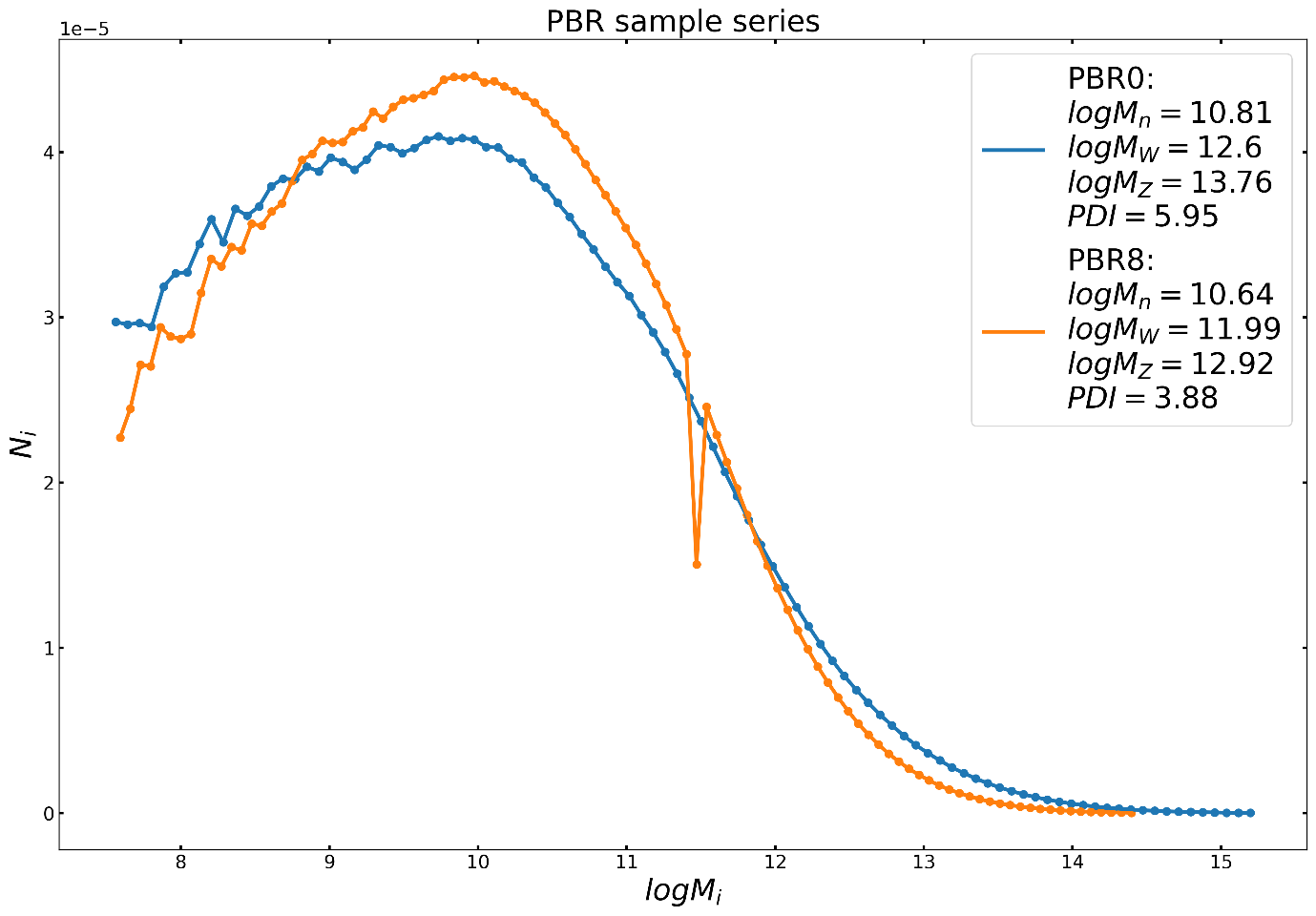
|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Sample | Mn | Mw | Mz | PDI |
| PAR0 | 48574.56 | 459847.2 | 1.81E+06 | 9.466832 |
| PAR5 | 42193.67 | 157422.4 | 4.01E+05 | 3.730948 |
| PBR0 | 49563.78 | 295124.7 | 9.50E+05 | 5.954444 |
| PBR8 | 41689.22 | 161689.9 | 4.07E+05 | 3.878458 |

Where:

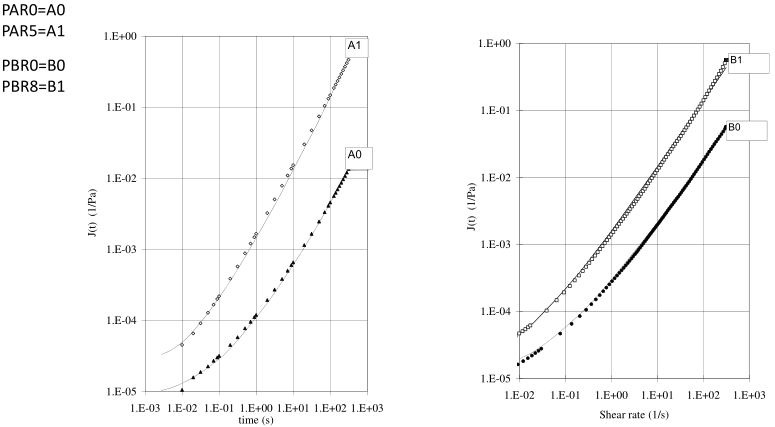
The MWDs are created from the number of molecules Ni of size Mi, where:

See calculations at <https://tecmx-my.sharepoint.com/:u:/g/personal/a01212611_itesm_mx/EcApVEoMr9JNooXyIt-d5p8BYIsvKZuTaMxFJnb6knlWIg?e=JLTsRl>



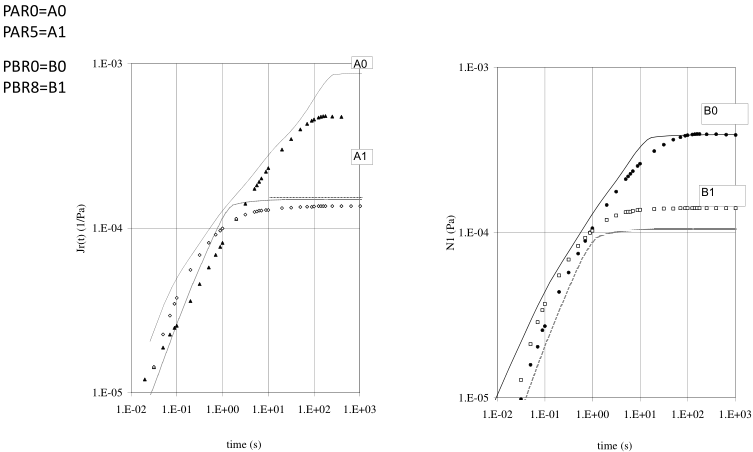


## Interpretation of the compliance modulus



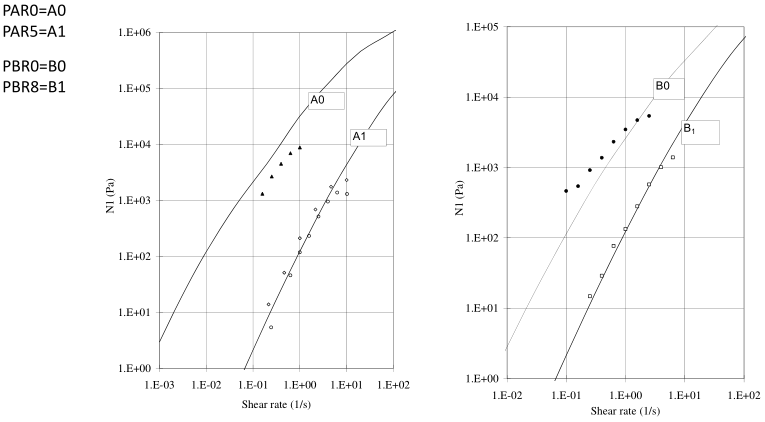
-If the polydispersity graph is narrower, then the creep compliance has a bigger slope and starts at a higher value in J(t) (compliance modulus). (Angel)

## The dependence of steady state compliance on molecular weight distribution



* The steady state compliance Je is a parameter that describes the chain elastic deformation capacity between entanglements (a.k.a. the accumulated deformation that is recoverable when the stress is removed)
* Je is dependent on molecular weight and on the width of the MWD, described by the PDI. As the stable state is reach at higher values with increasing PDI and Mn.
* The presence of these very high Mw should have an important impact in Je.
* The steady state value is reached earlier in narrower distributions (low PDI). [1]

## Correlation between the Normal stress difference and the MWD



- Normal stress difference (N1) upon increasing shear rate (cons)

REFERENCES

[1] J. Otegui, J. Ramos, J.F. Vega, J. Martínez-Salazar, Effect of high molar mass species on linear viscoelastic properties of polyethylene melts, Eur. Polym. J. 49 (2013) 2748–2758. https://doi.org/10.1016/j.eurpolymj.2013.06.015.