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Modelling Two Different Disperse Polystyrene with Maxwell Fractional Model in SAOS Experiments

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It is concluded in this work that Maxwell fractional model is able to describe the behaviour when Mw/Mn is closer to 1 but the same is not completely valid for polydispersity index of 1.44.

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I. Introduction

The purpose of this work is to perform two adjustments using the technique of Alves (Alves, 2017) with the data present in Farias (Farias, 2009) that belongs to a group of eminent researchers.

On this work is checked a possible correlation of the polydispersity index with the chain branching thanks to the realisation of adjustments of SAOS dynamic polystyrene data (Farias, 2009) with a mathematical formulated viscoelastic fractional model, the Maxwell fractional model(Jaishankar & McKinley, 2012).

Seeing the complexity level of Maxwell fractional model, is known that models on the literature can be more or less complex and divided in Newtonian (as Newton model)(Pinho, 2003), non-Newtonian inelastic (they are models that consider the variation of shear viscosity with shear rate) (Pinho, 2003)and viscoelastic (Viscoelastic models combine viscous component and elastic component and they can have differential or integral mathematical formulations)(Pinho, 2003).

First viscoelastic linear models date from XIX century and are the linear viscoelastic model of Maxwell (Maxwell, 1867) and the linear viscoelastic model of Kelvin-Voight (Bird, Armstrong, & Hassanger, 1987). A possible representation of this genre of models is given by the combination of discrete elements as springs (Hooke Law), where tension (τ) is directly proportional to deformation (γ)) to represent the elastic model, and dashpots (Newton law) (Bird et al., 1987).

With Fractional Viscoelastic models, an analogy with discrete elements can be done. On Figure 1 is presented this new element, the "springpot", that allows the interpolation of the behaviour of traditional elements spring and dashpot through the order considered for the derivative. In this way is obtained a continuous variation between the behaviour of solids and liquids. Hooke law (spring – derivative of order 0 (D^0)) and Newton law (dashpot – derivative of order 1 (D^1)) becomes a particular case of springpot (Friedrich, Schiessel, & Blumen, 1999).

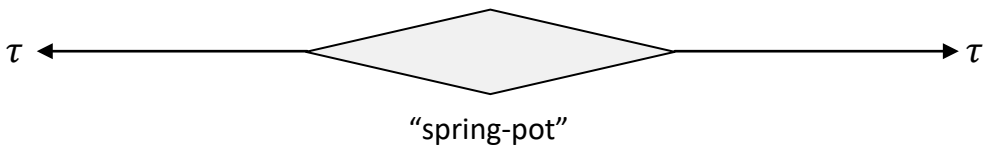

Figure 1: "Spring-pot" as generalization of the concept Spring-dashpot.

Below are presented the Equation 1, G'(ω), and the Equation 2, G''(ω),, equations of storage modulus, and Loss modulus of Maxwell fractional model (a model constituted by two springpot in series). These equations are used to fit the data of Farias.

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$$G'(\omega)=\frac{(\Phi_2\omega^{\beta})^2\Phi_1\omega^{\alpha}Cos\left(\frac{\pi}{2}\alpha\right)+(\Phi_1\omega^{\alpha})^2\Phi_2\omega^{\beta}Cos\left(\frac{\pi}{2}\beta\right)}{(\Phi_1\omega^{\alpha})^2+(\Phi_2\omega^{\beta})^2+2\Phi_1\omega^{\alpha}\Phi_2\omega^{\beta}Cos\left(\frac{\pi}{2}(\alpha-\beta)\right)} \quad \text{(Equation 1)}$$

$$G''(\omega)=\frac{(\Phi_2\omega^{\beta})^2\Phi_1\omega^{\alpha}Sin\left(\frac{\pi}{2}\alpha\right)+(\Phi_1\omega^{\alpha})^2\Phi_2\omega^{\beta}Sin\left(\frac{\pi}{2}\beta\right)}{(\Phi_1\omega^{\alpha})^2+(\Phi_2\omega^{\beta})^2+2\Phi_1\omega^{\alpha}\Phi_2\omega^{\beta}Cos\left(\frac{\pi}{2}(\alpha-\beta)\right)} \quad \text{(Equation 2)}$$

The Maxwell Fractional model to be valid must be > 0 for Φ_2 and Φ_1, and for α and β the observation of the final result is 0 < α and β <1 (Jaishankar & McKinley, 2012).

Fractional theory is not applied only in viscoelasticity.

This theory is applied on migration of biological cells in complex spatial domains (Cusimano, Burrage, & Burrage, 2013), on lithium-ion batteries involving fractional differentiation (Sabatier, Merveillaut, Francisco, Guillemard, & Porcelatto, 2014), on spiny neuronal dendrites (Henry, Langlands, & Wearne, 2008), on human motion tracking (Michailas, Martin, Lasse, & Manoli Yiannos, 2014) and also on fractional order cancer (Ahmed, Hashis, & Rihan, 2012).

On an engineering level these models can be applied on continuum mechanics (Drapaca & Sivaloganathan, 2012), on the optimization of fractional order dynamic chemical processing systems (Flores-Tlacuahuac & Biegler, 2014), on supercapacitors, batteries and fuel cells (Freeborn, Maundy, & Elwakil, 2015).

II. Resources and Techniques

On this work itis used data that Farias presented on her work (Farias, 2009), gently given by a group of eminent researchers and presented in work as "Evaluation of Reptation Model for predicting the linear viscoelastic properties of entangled linear polymers" (Ruymbeke, Keunings, Hagenaars, & Bailly, 2002) and also "Determination of the molecular weight distribution of the entangled linear polymers from linear viscoelasticity data" (Ruymbeke et al., 2002). As seen on table 1, there are 2 different polystyrene synthesized by anionic polymerisation and free radical polymerisation tested at 170 °C (Farias, 2009) with different polydispersity index.

Their characteristics are presented on Table 1.

Table 1: Characteristics of the Polystyrenes used on this work

	Mw (g/mol)	Mw/Mn	Test temperature °C
Anionic Polymerisation PS (PS_a)	355500	1.03	170
Free-radical Polymerisation PS (PS_f)	361100	1.44	170

These two Polystyrenes were analysed according to Farias on a rotational rheometer ARES (Advanced Rheometric Expansion System) of controlled deformation throughout dynamic experiments with parallel plate geometry(Farias, 2009). The GPC (Gel Permeation Chromatography) gives the medium molar mass and the Polydispersity index with the help of a liquid chromatographer Waters Alliance model GPC 1 V2000 equipped with refraction index(Farias, 2009).

For more information it is necessary to consult two works, the "Evaluation of Reptation Model for predicting the linear viscoelastic properties of entangled linear polymers" (Ruymbeke et al., 2002) and also the "Determination of the molecular weight distribution of the entangled linear polymers from linear viscoelasticity data" (Ruymbeke et al., 2002).

This data of G'(ω) and G''(ω) of SAOS experiments was placed on a computer program previous computed by Alveswhich is possible to be found on the article website (Alves, 2017), using the same principle. Alves modified the file .cdf of Normand et al. (Normand, Eisenberg, & Peleg, 2012)used to evaluate a stochastic model inactivation for heat activation spores of Bacillus spp (Corradini, Normand, Eisenberg, & Peleg, 2010)and converted it into a .cdf file to perform adjustment of fractional viscoelastic data. The file .cdf is easily modified if replaced the equation and the dataset.

III. Results and Discussion of Results

The results of the work are presented on Table 2 for Maxwell fractional model adjustment to the experimental SAOS dynamic experimental data of Farias.

Table 2: Maxwell Fractional Model results of adjustment for the different PS used in this work

	Φ_1	Φ_2	α	β	R^2
Anionic Polymerisation PS (PS_a)	1029000	132900	0.987	0.120	0.9987
Free-radical Polymerisation PS (PS_f)	275800	116400	0.842	0.126	0.990

Accordingly to parameters values is observed that all values are >0 for Φ_2 and Φ_1, which means that in this case it obeys the thermodynamic restrictions. Therefore, for α and β the observation of the final result is 0< α and β<1, which gives valid thermodynamic results.

Below are presented the graphics of the adjustments done with the material functions G'(ω) and G''(ω) of Maxwell Fractional Model with the experimental data of Farias, the anionic polymerisation data of Polystyrene (Figure 2) and free-radical polymerisation data of Polystyrene (Figure 3).

Figure 2 shows an almost perfect adjustment for G'(ω) and G''(ω) in all the domain of ω with exception for ω>200 rad/s. For this value the result is not perfectly coincident, and means that the model is not valid for values of ω>200 rad/s.

On Figure 3 is observed the same thing as Figure 1 but here for values of ω>100 rad/s, which results on a bad coincidence result. Here, also for periods of ω<0.05 rad/s relative to G'(ω) and G''(ω) the fit is not good.

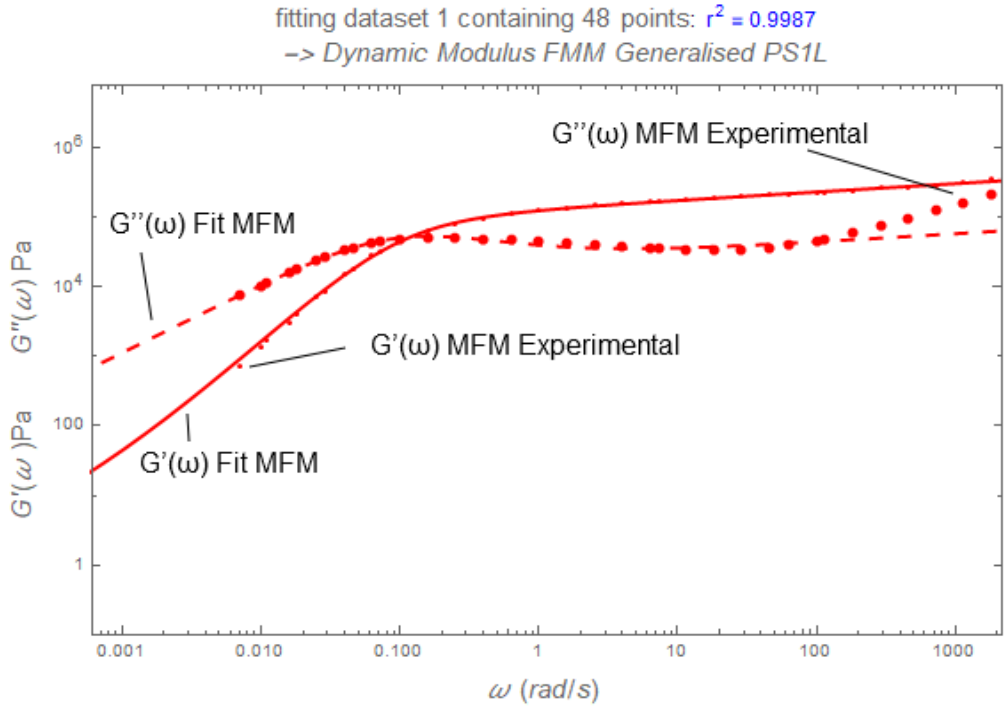

Figure 2: Maxwell Fractional Model adjustment for SAOS experimental data of an anionic Polymerisation PS

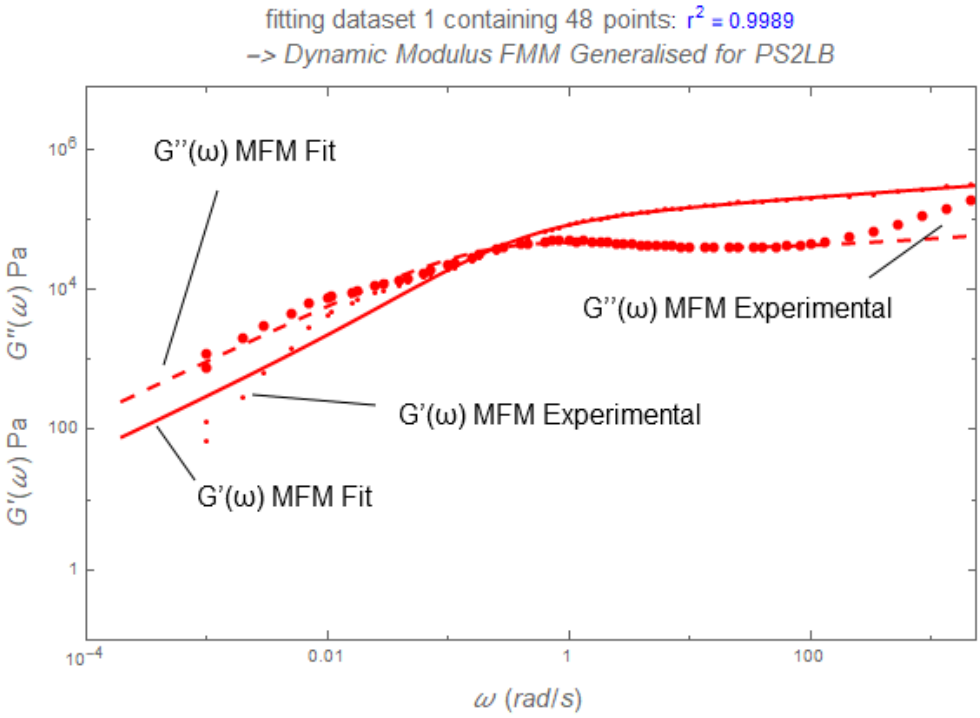

Figure 3: Maxwell Fractional Model adjustment for SAOS experimental data of an free-radical polymerisation PS

Although, the final results in questions of adjusted R squared are very high, and this results in a good model to adjust these experimental data in SAOS experiments.

The anionic polymerized polystyrene as observed on section 5 has polydispersity index correspondent to 1.03 adjusting almost perfectly, which means that exist an high correlation between Maxwell fractional model and the polydispersity index of anionic polymerised polystyrene.

The free radical polymerization Polystyrene has a bigger polydispersity index equal to 1.44 and the quality of adjustment is not comparable to the anionic polymerisation of polystyrene, what means that for Mw = 1.44 Mn the correlation between Maxwell fractional model and polydispersity index of free radical based polymerisation cannot be done.

So, I think that with these proofs that the overall quality of Maxwell fractional model has a correlation with polydispersity index for anionic polymerisation polydispersity index however the same is not completely valid for free-radical based polymerisation of polystyrene.

IV. Conclusion

With this work was possible to perform two fits for two different polystyrenes with an overall good quality obeying the thermodynamic restrictions imposed by Maxwell Fractional Model in SAOS dynamics.

However is possible to find now a correlation with the polydispersity index of the polymer of Polystyrene with the Maxwell fractional model.

It is concluded in this work that Maxwell fractional model is able to describe the behaviour when Mw/Mn is closer to 1 but the same is not completely valid for polydispersity index of 1.44.

V. Acknowledgements

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