

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

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Abstract

The purpose of this work is to perform two adjustments of different disperse polystyrene using the technique of Alves (Alves, 2017) with the data present on Farias (Farias, 2009), data belonging to a group of eminent researchers. It is seen that the adjustments are of good quality for a polystyrene anionic polymerised and with an inferior quality for a free-radical polymerised polystyrene. It leads to a possible correlation with the polydispersity index and the quality of adjustment performed with Maxwell fractional model. It is concluded in this work that Maxwell fractional model is able to describe the behaviour when M_w/M_n is closer to 1 but the same is not completely valid for polydispersity index of 1.44.

Index terms— Maxwell fractional model; viscoelastic fluid; SAOS experiments; polystyrene; wolfram mathematica 10; non-linear regression; polydispersity index.

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

Bruno Manuel Ribeiro Alves I. Introduction the purpose of this work is to perform two adjustments using the technique of Alves (Alves, 2017) with the data present on 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 (?) is directly proportional to deformation (?) 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 ?? 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 (Abstract-The purpose of this work is to perform two adjustments of different disperse polystyrene using the technique of Alves (Alves, 2017) with the data present on Farias ??Farias, 2009), data belonging to a group of eminent researchers. It is seen that the adjustments are of good quality for a polystyrene anionic polymerised and with an inferior quality

44 for a free-radical polymerised polystyrene. It leads to a possible correlation with the polydispersity index and
 45 the quality of adjustment performed with Maxwell fractional model.

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

48 **2 Keywords: Maxwell fractional model; viscoelastic fluid;**
 49 **SAOS experiments; polystyrene; wolfram mathematica 10;**
 50 **non-linear regression; polydispersity index.**

51 **3 ??**

52 "spring-pot" $\gamma(t) = \sum_{i=1}^n G_i \cos(\omega t - \delta_i)$ $\gamma(t) = \sum_{i=1}^n G_i \cos(\omega t - \delta_i)$ $\gamma(t) = \sum_{i=1}^n G_i \cos(\omega t - \delta_i)$
 53 $\gamma(t) = \sum_{i=1}^n G_i \cos(\omega t - \delta_i) + \sum_{i=1}^m G_i \sin(\omega t - \delta_i) = \sum_{i=1}^n G_i \cos(\omega t - \delta_i) + \sum_{i=1}^m G_i \sin(\omega t - \delta_i)$ (Equation 1) $\gamma(t) = \sum_{i=1}^n G_i \cos(\omega t - \delta_i)$
 54 $\gamma(t) = \sum_{i=1}^n G_i \cos(\omega t - \delta_i) + \sum_{i=1}^m G_i \sin(\omega t - \delta_i) = \sum_{i=1}^n G_i \cos(\omega t - \delta_i) + \sum_{i=1}^m G_i \sin(\omega t - \delta_i)$
 55 $\gamma(t) = \sum_{i=1}^n G_i \cos(\omega t - \delta_i) + \sum_{i=1}^m G_i \sin(\omega t - \delta_i) = \sum_{i=1}^n G_i \cos(\omega t - \delta_i) + \sum_{i=1}^m G_i \sin(\omega t - \delta_i)$ (Equation 2)

56 Fractional theory is not applied only in viscoelasticity. This theory is applied on migration of biological cells
 57 in complex spatial domains (Cusimano, Burrage, & Burrage, 2013), on lithium-ion batteries involving fractional
 58 differentiation ?? On an engineering level these models can be applied on continuum mechanics (Drapaca &
 59 Sivaloganathan, 2012), on the optimization of fractional order dynamic chemical processing systems (Flores-
 60 Tlacuahuac & Biegler, 2014), on supercapacitors, batteries and fuel cells (Freeborn, Maundy, & Elwakil, 2015).
 61 For more information it is necessary to consult two works, the "Evaluation of Reptation Model for predicting the
 62 linear viscoelastic properties of entangled linear polymers" (Ruymbeke et al., 2002) and also the "Determination
 63 of the molecular weight distribution of the entangled linear polymers from linear viscoelasticity data" (Ruymbeke
 64 et al., 2002).

65 **4 II. Resources and Techniques**

66 This data of $G'(\omega)$ and $G''(\omega)$ of SAOS experiments was placed on a computer program previous computed by
 67 Alves which is possible to be found on the article website (Alves, 2017), using the same principle. γ , which means
 68 that in this case it obeys the thermodynamic restrictions. Therefore, for γ and δ the observation of the final
 69 result is $0 < \gamma < 1$ and $\delta < 1$, which gives valid thermodynamic results.

70 Figure 2 shows an almost perfect adjustment for $G'(\omega)$ and $G''(\omega)$ in all the domain of ω with exception for
 71 $\omega > 200$ rad/s. For this value the result is not perfectly coincident, and means that the model is not valid for
 72 values of $\omega > 200$ rad/s. On Figure 3 is observed the same thing as Figure ?? but here for values of $\omega > 100$ rad/s,
 73 which results on a bad coincidence result. Here, also for periods of $\omega < 0.05$ rad/s relative to $G'(\omega)$ and $G''(\omega)$ the
 74 fit is not good.

75 Below are presented the graphics of the adjustments done with the material functions $G'(\omega)$ and $G''(\omega)$ of
 76 Maxwell Fractional Model with the experimental data of Farias, the anionic polymerisation data of Polystyrene
 77 (Figure 2) and free-radical polymerisation data of Polystyrene (Figure 3). The anionic polymerized polystyrene as
 78 observed on section 5 has polydispersity index correspondent to 1.03 adjusting almost perfectly, which means that
 79 exist an high correlation between Maxwell fractional model and the polydispersity index of anionic polymerised
 80 polystyrene.

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

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

88 **5 IV. Conclusion**

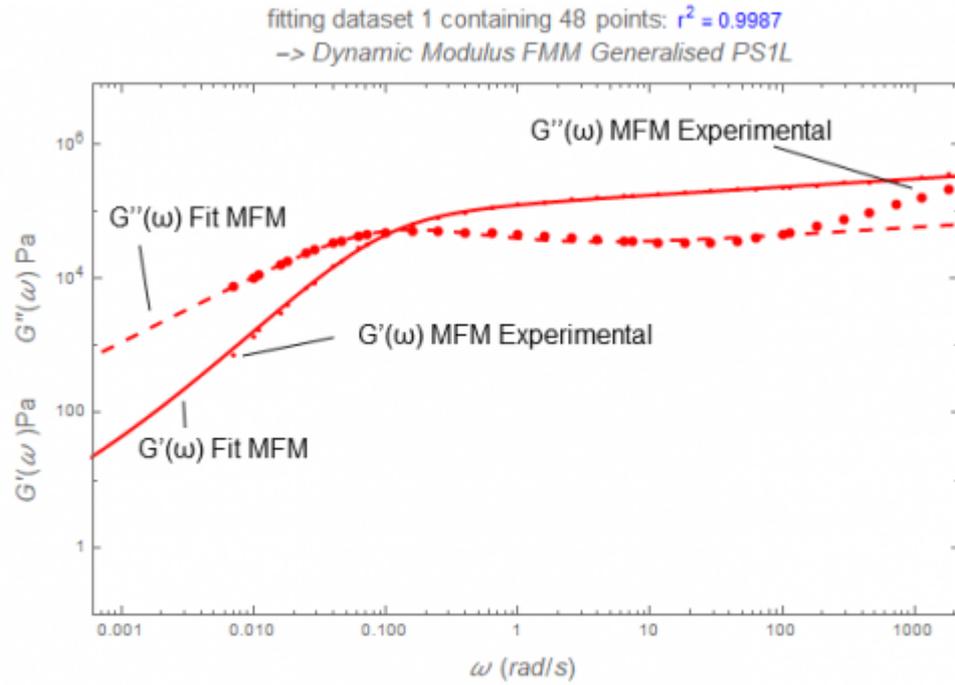
89 With this work was possible to perform two fits for two different polystyrenes with an overall good quality obeying
 90 the thermodynamic restrictions imposed by Maxwell Fractional Model in SAOS dynamics. However is possible
 91 to find now a correlation with the polydispersity index of the polymer of Polystyrene with the Maxwell fractional
 92 model.

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

95 **6 V. Acknowledgements**

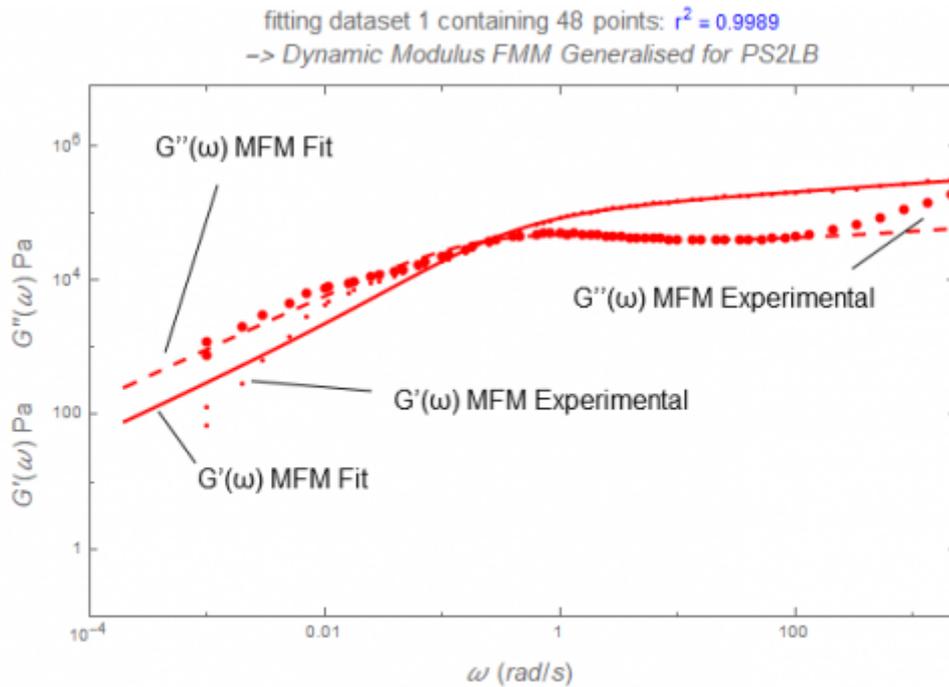
96 The present work has got the software funding of Wolfram Software Mathematica 10.4. ¹

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Figure 1: 0D 1 D 2017 JFigure 1 :



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Figure 2: Figure 2 :

Figure 3:

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	Mw (g/mol)	Mw/MfTest	tem- per- a- ture °C
Anionic Polymerisation PS (PS a) Free-radical Polymerisation PS (PS f)	355500	1.03	170
	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).

Figure 4: Table 1 :

Year 2017 The Maxwell Fractional model to be valid must be > 0 for 2α and $1 - \alpha$, and for α and β the observ

30 of the final result is $0 < \alpha$ and $\beta < 1$ (Jaishankar & McKinley, 2012).

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Global (Ruymbeke, Keunings, Hagenaaars, & Bailly, 2002) and also "Determination of the molecular weight
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by anionic polymerisation
polymerisation tested at 170 °C (Farias, 2009) with
different polydispersity index.
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Figure 5:

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Accordingly to parameters values is observed
that all values are >0 for 2α and $1 - \alpha$

Figure 6: Table 2 :

Figure 7:

Figure 8:

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