Comparison of Viscoelastic Moduli Fitting Using Optimization Methods

F. Pelayo[a], A. Noriega[b], M.J. Lamela[c], A. Fernández-Canteli[d]

Department of Construction and Manufacturing Engineering. University of Oviedo

Campus de Viesques. 33203 Gijón. Spain

[a]fernandezpelayo@uniovi.es, [b]noriegaalvaro@uniovi.es, [c]mjesuslr@uniovi.es, [d]afc@uniovi.es

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Abstract. Usually, viscoelastic models based on Prony's series are used to fit the master curves from experimental results. However, the fitting process requires previous knowledge of the time-parameters of the model, τ_i, in order to fit the corresponding modulus. In general, a homogeneous distribution in logarithmic-time scale is used for τ_i, but a large number of terms in the Prony's series are needed to achieve a suitable fitting that cannot be implemented into a commercial finite element code, in which the number of terms can be limited.

As an alternative, a new optimizing methodology for fitting master curves of viscoelastic materials with Prony-based models is presented. This approach can be applied to the definition of different experimental viscoelastic master curves, such as those related to relaxation or creep. Finally, the results are compared with those obtained with the homogeneous distribution fitting method.

Introduction

The viscoelastic behaviour is a function of time and temperature. This dependence requires, in general, the definition of a set of master curves at different temperatures to fully characterize the material under all possible working and failure conditions. These master curves can be obtained experimentally [1, 2] or by means of viscoelastic interconversions [3, 4]. Anyway, in both cases the experimental data must be fitted to a viscoelastic model, e.g. Prony series [5], in order to carry out further calculations with the viscoelastic material.

With this proposal, several methods, such as the Procedure X [6, 7], the collocation method [8], the Multidata method [9] or the Emri and Tschoegl iterative algorithm [10, 11] are mainly used to obtain the viscoelastic model coefficients, e.g. (e_i, τ_i) and (d_p, τ_p) that determinate the discrete relaxation and retardation spectrums, respectively, that define the viscoelastic material behaviour.

The basis of the methods consists in establishing a set of discrete times and them fitting with different criteria the rest of the model coefficients. However as the experimental data are usually acquired at logarithmic sampling and, also the viscoelastic function of the material covers several logarithmic decades, the methods select the discrete times (τ_i or τ_p) in some way that finally are equally spaced on the logarithmic time axis (homogeneous distribution). Although some of these method presents some inconveniences in the fitting process, such as, negative spectral lines, in general good fittings can be achieved reducing the discrete times space or, that it is the same, increasing the number of terms in the corresponding Prony series. However when the viscoelastic model is used for further calculations, such as, finite elements (FE) simulations, a few or reduced number of terms are necessary or preferable, e.g., FE codes that limit the number of terms to be used, modal updating of structures or components with viscoelastic materials or simply for reducing computational time.

In this work, a new method for fitting viscoelastic experimental functions, such as relaxation or retardation including the possibility of a non-homogeneous distribution of discrete times on the logarithmic time axis, is proposed. The model is validated using experimental relaxation curves of PVB (Polyvinyl butiral) and the results are compared with those obtained by homogeneous times distribution.

Theory

Viscoelastic Behaviour and Models. Viscoelastic materials can be, in a simple way, understood like those materials whose properties are somewhere between elastic solids and Newtonian fluids. Although its real behaviour is, in general, more complex, this point of view allows an easier understanding of the viscoelastic mathematical models for these kind of materials. Both elastic solid and Newtonian fluid behaviour are each one represented by springs and dashpots, respectively, so viscoelastic materials can be represented with combinations of springs and dashpots. The simplest models are the Maxwell and Kelvin Model, where the first one (with elements in series) is used for representing relaxation viscoelastic functions, $E(t)$, while the second one (with elements in parallel) is used for representing creep viscoelastic functions, $D(t)$, [12, 13, 14]. When dealing with real materials the obtained results with these simpler models can be not satisfactory so the generalized versions of the previous ones, that have several Maxwell or Kelvin models connected, must be used. To fit experimental data with the generalized models, these are usually represented by means of Prony series where each term of the series is identify with one individual Maxwell or Kelvin model. The Prony series for the generalized Maxwell model is

$$E(t) = E_0 \left[1 - \sum\nolimits_{i=1}^{n_t} e_i \left(1 - \exp\left(-\frac{t}{\tau_i}\right)\right)\right] \tag{1}$$

where E_0 is the glassy modulus, n_t the number of Maxwell terms and (e_i, τ_i) the Prony coeficients (e_i is the discrete spectral line value at relaxation time τ_i).
The corresponding Prony series for the generalized Kelvin model is given by

$$D(t) = D_0 \left[1 + \sum\nolimits_{p=1}^{m_t} d_p \left(1 - \exp\left(\frac{t}{\tau_p}\right)\right)\right] \tag{2}$$

where D_0 is the glassy compliance, m_t the number of Kelvin terms and (d_p, τ_p) the Prony coeficients (d_p is the discrete spectral line value at retardation time τ_p).

Homogeneous Distribution Model Fitting. To use the previous models with real viscoelastic materials, data from experiments must be fitted in order to obtain the Prony series coeficients, e.g. (e_i, τ_i) for relaxation functions. To introduce and derive the optimizing method, relaxation Prony model (eq. (1)) is used (the same fitting process can be directly applied to the retardation model).

The first step is to establish the maximum number of terms, n_{max}, that could be used in the fitting process. Then, for each group of terms ($n_{t=1:max}$), that is, a series with one term, a series with two terms, and so on, until n_{max} terms will be used, a prony series is fitted to the experimental data using equal spaced times, τ_i, in logarithmic time axis as follows:

$$\tau_i = \tau_{min} + \frac{\tau_{max} - \tau_{\min}}{n_t + 1} \cdot i \tag{3}$$

where $\tau_{min} = \min(\tau_k)$, $\tau_{max} = \max(\tau_k)$ and $k = 1{:}\, r$ are the number of experimental data.

Once τ_i are defined, value of $E(\tau_i)$ is obtained, e.g. by a cubic spline interpolation from experimental data. Next, a linear system of n_t equations can be formed as follows

$$\sum\nolimits_{i=i}^{n} e_i \cdot A_{ij} = b_j; \qquad j = 1, \cdots, n-1 \tag{4}$$

$$\sum\nolimits_{i=1}^{n} e_i = \frac{E_0 - E_\infty}{E_0} \tag{5}$$

where

$$A_{ij} = 1 - \exp\left(-\frac{\tau_j}{\tau_i}\right) \tag{6}$$

$$b_j = 1 - \frac{E(t_j)}{E_0} \tag{7}$$

and E_∞ is the equilibrium modulus. In order to assess the error in the fitting process with the homogeneous time distribution, the following indicator, S_{homog}, is used

$$S_{homog} = \sum\nolimits_{k=1}^{r} \left(E(t_k) - E_{Prony}(t_k)\right)^2 \tag{8}$$

Optimal Distribution Model Fitting. Similarly to the homogeneous distribution, for each previous fitted model, a second Prony series is fitted but, in this case, the time coefficients, τ_{i-opt} , are optimally distributed so that a minimum is required in the next error indicator

$$S_{opt} = \sum\nolimits_{k=1}^{r} \left(E(t_k) - E_{Prony}(t_k, \vec{\tau})\right)^2 = f(\vec{\tau}) \tag{9}$$

To obtain this optimal distribution, the next posed optimization problem is to set out

$$\begin{gathered} \min(S_{0pt}) \\ \tau_i \in [\tau_{min}, \tau_{max}] \end{gathered} \tag{10}$$

where $E_{Prony}(t_k, \vec{\tau})$ depends on vector $\vec{\tau}$ that contains the n_t values of τ_{i-opt}. To solve the optimizing problem, firstly A_{ij} and b_j must be obtained with eqs. (6) and (7), respectively, and then,

E_{prony} is calculated. Next, the linear system of eq. (4) and (5) is solved in order to obtain the values of e_{i-opt}.

The optimization problem sets out in eq. (10) has the following characteristics:

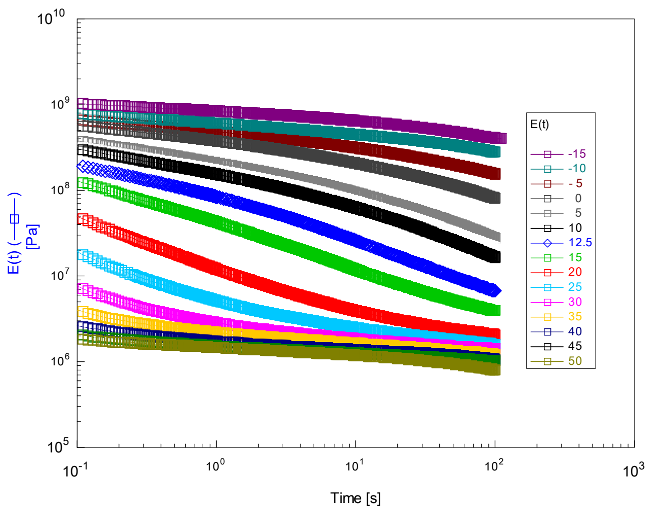
- *Single-objective problem.*
- *The variables are continuous and bounded.*

With these features and taking into account that an efficient algorithm is needed, since the commented process is repeated for each value of n_t, the Discrete Directions Mutation Evolutive Strategy (DDM-ES) [15] is selected because it has a behaviour and use similar to a genetic algorithm, therefore, less objective function evaluations and computational time is needed.

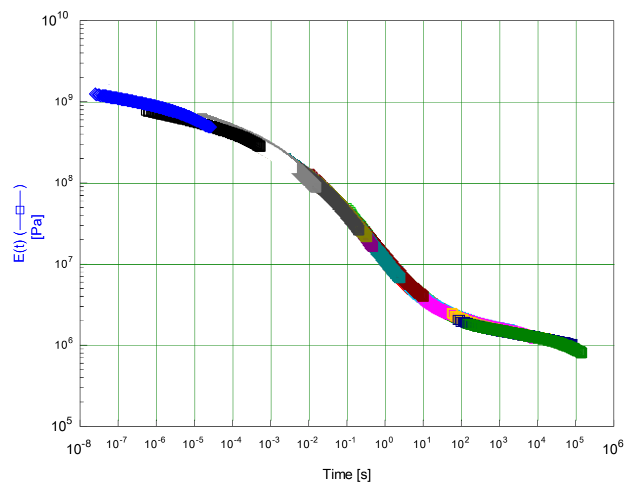
Experimental Program.
Material. The material used in the tests was PVB (Polyvinyl butiral), a thermoplastic material which shows a linear-viscoelastic behaviour [16]. The specimen dimensions were 25 x 5 mm approximately with a standard thickness of 0.38 mm.

Equipment. A DMA RSA3 of T.A. Instruments was used for testing. The equipment has a temperature-controlled oven that permits a wide range of temperatures from -50 ºC to 150 ºC. A special tensile fixture for small dimensions specimens was used in the tests.

Experimental viscoelastic functions of the material. From short-time relaxation curves (10e-1 to 10e2 seconds) at different temperatures, see Fig. 1a), a broad-time master curve (10e-7 to 10e6 seconds) can be constructed for the material, see Fig. 1b), using the Time-Temperature Superposition Principle (TTS) by means of the William-Landel-Ferry model (WLF) [17]. In this work, the reference temperature was chosen at $T_0 = 20\ ºC$ and the obtained WLF constants for the material were C1=12.6027 and C2=74.46, respectively.



a)



b)

Fig. 1. a) Curves of PVB at different temperatures and b) Master curve of PVB for a reference temperature of 20 ºC.

Analysis of Results.

Fitting the material master curve shown in Fig. 1b) with both homogeneous and optimal time distributions, see Table 1, for $n_t = 10$, a plot of the squared error for each case, eqs. (8) and (9), respectively, can be constructed as presented in Fig. 2.

Table 1. Parameters used in the DDM-ES process for optimal times distribution [12].

$\Delta\sigma = 10$	$Popsize = 50$	$iii = 0$
$\Delta n_{ii} = 1$	$n_{dv} = 3$	$g = 30$

From the values of the squared error calculated in function of the number of terms used in the Prony series, it can be inferred that the optimal distribution of times generates a smaller squared error than the homogeneous distribution. As it can be seen in Fig. 2, this difference is maintained in logarithmic scale if the number of terms in the series increases.

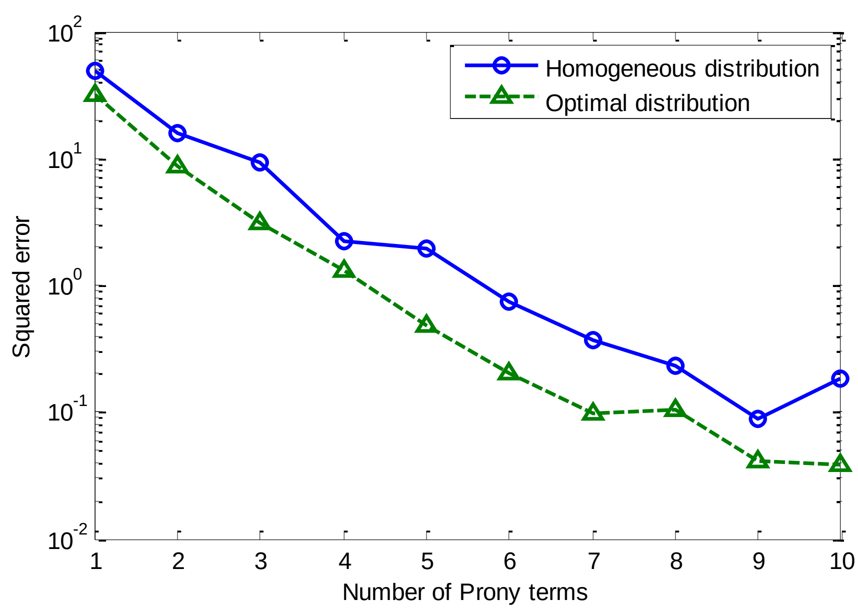


Fig. 2. Variation of the fit goodness for PVB master curves using homogeneous and optimal distributions with different number of Prony terms.

As a consequence, with an optimal distribution can be obtain similar squared error values to those obtained with a homogeneous distribution but using less terms in the series. For example, the square error of the optimal distribution with 6 terms is similar to the homogeneous distribution with 8 terms.

If the fitted model with optimal and homogeneous distribution, respectively, are represented together with the experimental data, see Figure 3, it can be noticed that the solution with optimal distribution gives a better fitting to the experimental data than the obtained with the homogeneous distribution.

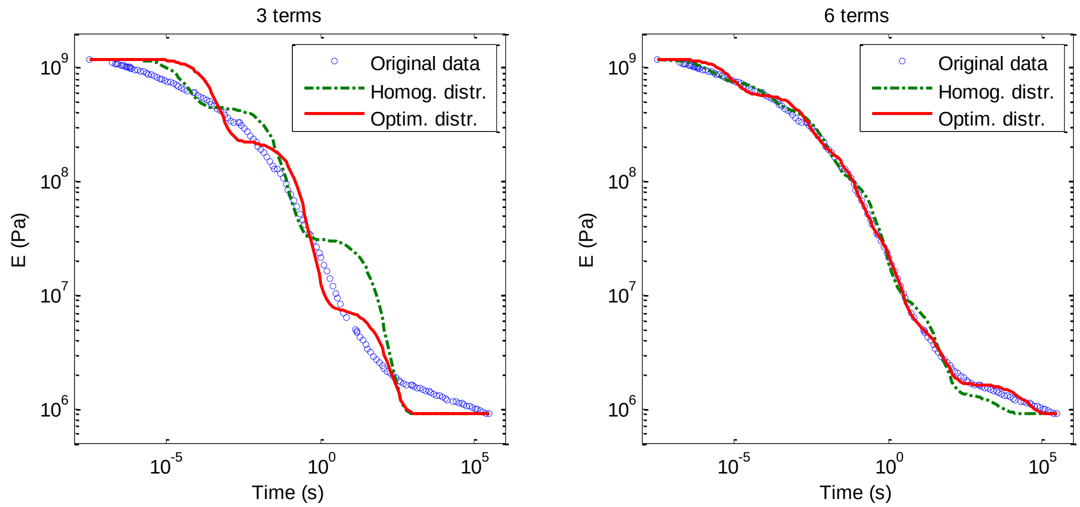


Fig. 3. Comparison of the PVB master curve using homogeneous and optimal distributions of the experimental data fitted by Prony series with 3 and 6 terms.

On the other hand, if one of the short-time viscoelastic relaxation curves is fitted using both procedures, Fig. 4 shows as the homogeneous distribution squared error increases with the number of terms used in the Prony series, whereas the optimal distribution error presents the same tendency than in the material broad-time curve (master curve). Comparing the square error for homogeneous and optimal distributions, it is remarkable the large difference of values obtained between them.

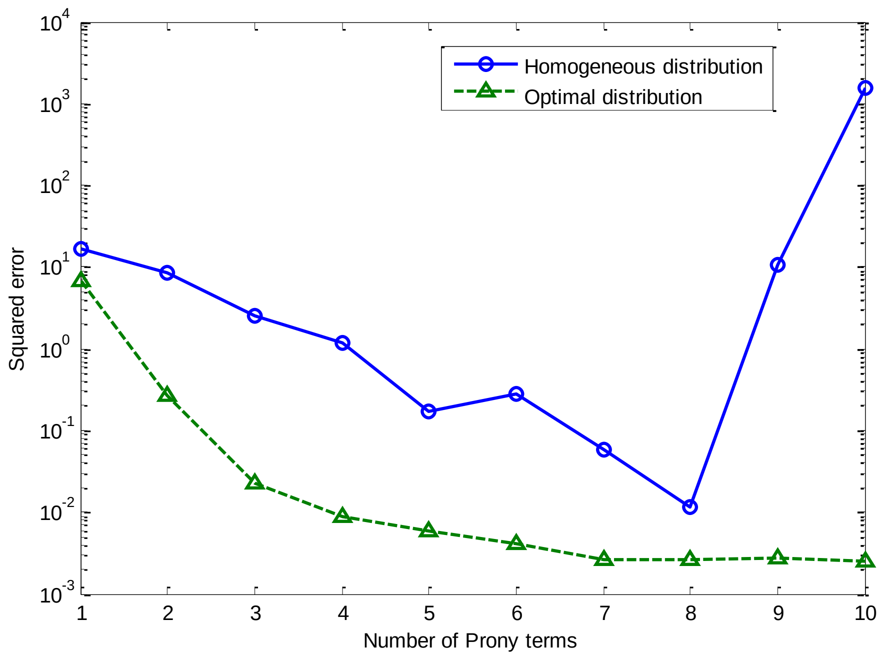


Fig. 4. Variation of the fit goodness for PVB short-time curves using homogeneous and optimal distributions with different number of Prony terms.

In Fig. 5 are presented the Prony series models with 3 and 6 terms, respectively, obtained with homogeneous and optimal time distribution. In this case, the Prony series with 3 terms fitted with optimal distribution is in good agreement with the experimental data (see Fig. 5), while 8 terms are needed in the homogeneous distribution fitting for obtained the same results and error (see Fig. 4).

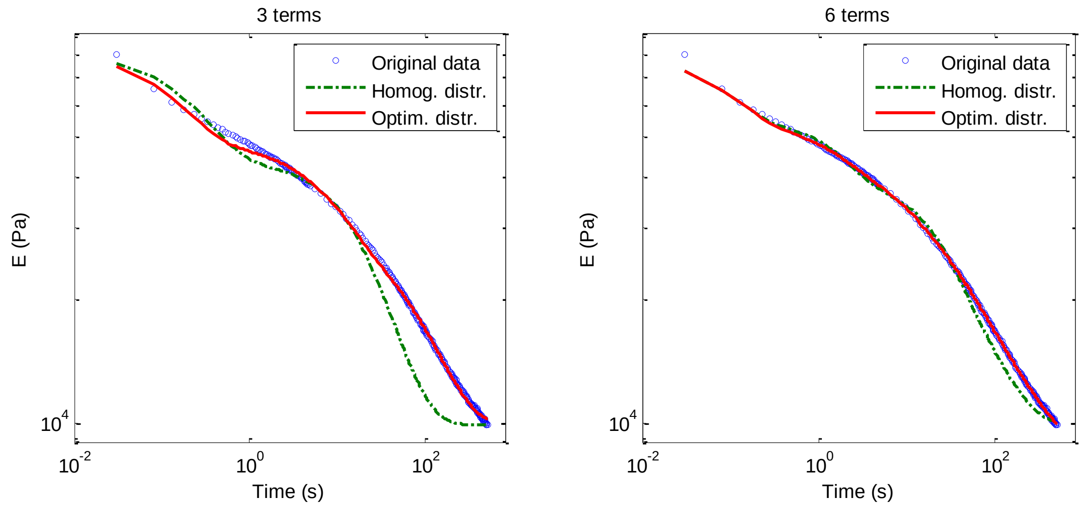


Fig. 5. Comparison of the PVB short-time curves using homogeneous and optimal distributions of the experimental data fitted by Prony series with 3 and 6 terms.

Conclusions

- A new methodology to achieve the optimal discrete time distribution, τ_i, in viscoelastic model fittings based on Prony series is developed.
- Using an optimal time distribution leads to more accurate results than those obtained from a homogeneous time distribution.
- Short-time viscoelastic curves provide larger error differences between homogeneous and optimal distributions than in broad-time curves, so the use of an optimal time distribution is recommended.
- Prony series with less number of terms guarantee good accuracy when using an optimal time distribution, thus facilitating subsequent material modeling, for instance, in FE analysis.

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