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BAYESIAN CHARACTERIZATION OF FRACTIONAL DERIVATIVE MODEL PARAMETERS OF VISCOELASTIC MATERIALS

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Abstract. *Passive vibration control methods have made large use of viscoelastic materials, due to its high capacity to dissipate energy. The design of efficacious vibration control devices using viscoelastic materials requires detailed knowledge of the dynamic material behavior. That is, it is essential to identify precisely the dynamic properties, represented by the real modulus of elasticity and the corresponding loss factor. These properties are usually obtained by conducting an experiment in wide ranges of temperature and frequency, since the properties are dependent of these factors. Previous work demonstrated that variability in the dynamic properties is due to random rather than deterministic mechanisms. This paper proposes the use of Bayesian inference approach to characterize the parameters of a typical and well-known viscoelastic material. Results obtained on an specific experiment, where samples from the material were tested at different frequencies and temperatures, generated data for the investigation. The material is initially modelled, in the frequency domain, by a four parameter fractional derivative model. Subsequently, as the temperature is considered a source of variation for the model, the number of parameters is raised to six. Through the Bayesian approach, the collected data were used along with adequate prior distributions for the fractional derivative parameters, to simulate their posterior distribution by Monte Carlo*

Markov Chain (MCMC) methods. After applying diagnostics for checking the convergence of the MCMC, simulated values from the posterior distributions were summarized by histograms and descriptive statistics. It is shown that this framework enabled more accurate statistical inference about material properties.

Keywords: *Bayesian Inference, Posterior Distribution, Vibration Control, Viscoelastic Material.*

1 INTRODUCTION

Due to its energy dissipative characteristics, viscoelastic materials have been largely use in passive vibration control methods (Pritz, 2001). Thus application is broad and includes aerospatial and biomechanical components. However, the efficacious application of these materials in passive vibration control requires detailed knowledge about their dynamic behavior (Espíndola, et al., 2008). A well established way of describing the dynamic behavior of viscoelastic materials is through their complex modulus representation, since the complex notation brings together the elastic characteristics of the material, represented by the real modulus, and the dissipative characteristics, described by the imaginary modulus, or yet the corresponding loss factor. These are known as the dynamic properties of the viscoelastic material.

Dynamic properties will be modeled by the four-parameter fractional derivative model. That model proves to be a powerful tool in describing the dynamic behavior of real materials used for the passive vibration control (Bagley and Torvik, 1986; Pritz, 1996).

The dynamic properties are highly dependent on frequency and temperature. Therefore, dynamic characterization must consider wide ranges of frequencies and temperatures for proper characterization of the material behavior.

The experimental statistical variability associated to dynamic properties is close to 20% (Balbino, 2012) and the factors that are associated to this uncertainty are not controlled. Thus, it is important to employ mechanisms that can quantify the uncertainty during the identification of the properties. Currently, the method of least-squares error has been used for associating experimental data and the model prediction (Gogu et al., 2010). However, this method does not take into account the uncertainty in the identification of the dynamical properties due to measurement and modeling errors.

The objective of the present paper is to illustrate the Bayesian inference as a way of assessing the behavior of complex modulus by taking into account their uncertainty. Application of Bayesian inference is intended to incorporate into parameters estimates the model and measurement uncertainties by fitting a probability distribution for the complete identification of the viscoelastic material properties.

Zhang et al. (2013) and Hernandez et al. (2015) adopted this approach for identifying parameters of viscoelastic materials, considering, however, variable frequency and constant temperature. Both frequency and temperature dependencies are considered herein.

2 DYNAMIC CHARACTERIZATION

The viscoelastic materials, have in the frequency domain representation of the complex modulus, a well-known way of describing their dynamic behavior. The real and imaginary parts represent the elastic and dissipative characteristics, respectively. Thus, the complex Young's modulus $\overline{E}$ of a viscoelastic material can be written as

$$\overline{E} = E_R + iE_I \tag{01}$$

The loss factor η_E can be defined as the ratio between the imaginary modulus, E_I and real modulus, E_R, as

$$\eta_E = E_I/E_R \tag{02}$$

The loss factor is, therefore, associated with the mechanisms by which the material dissipate energy; the higher the energy dissipation, the higher the loss factor. Thus the, complex Young's modulus can be written as

$$\overline{E} = E_R\left(i + i\eta_E\right) \tag{03}$$

These equations are also valid, with the corresponding changes, for the shear modulus.

2.1 Effects of Temperature

The viscoelastic materials are influenced by external factors that have to be properly considered for the correct characterization of their dynamic behavior. According to Nashif et al. (1985), temperature is the most important external factor affecting the dynamic properties of viscoelastic materials. The temperature effect is illustrated in Fig. 1, that shows 3 main distinct regions and the behavior of a typical material in each one.

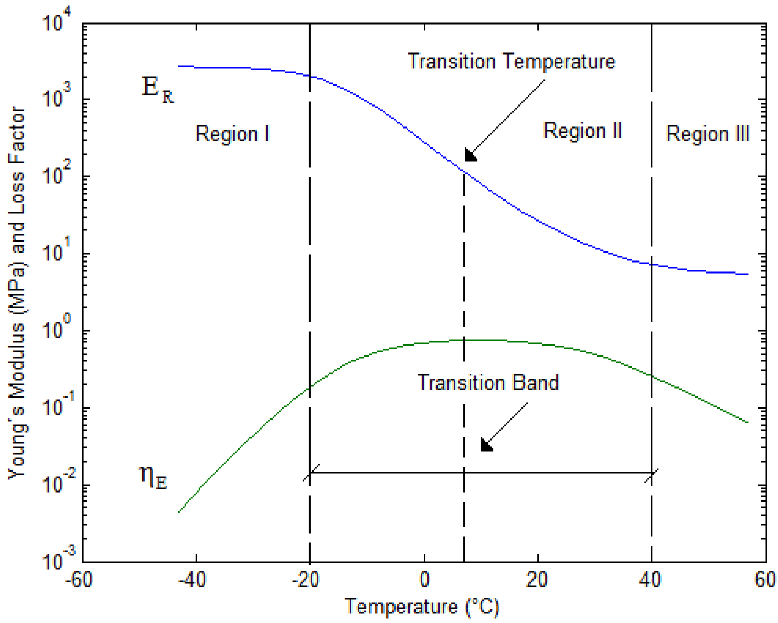

Figure 1 – Variation of E_R and η_E with temperature in a typical viscoelastic material.

2.2 Effects of Frequency

It is observed, in frequency, the real modulus always increases with the increasing frequency, even if slightly. The steepest increase occurs in the so called transition region (Nashif et al., 1985). When observing the loss factor behavior, it can be noticed that it initially increases with increasing frequency, reaches a maximum and then decreases. This behavior can be seen in Fig. 2, for a typical material. Comparing Figs. 1 and 2, it is observed that the frequency dependence is qualitatively inverse to the temperature dependence.

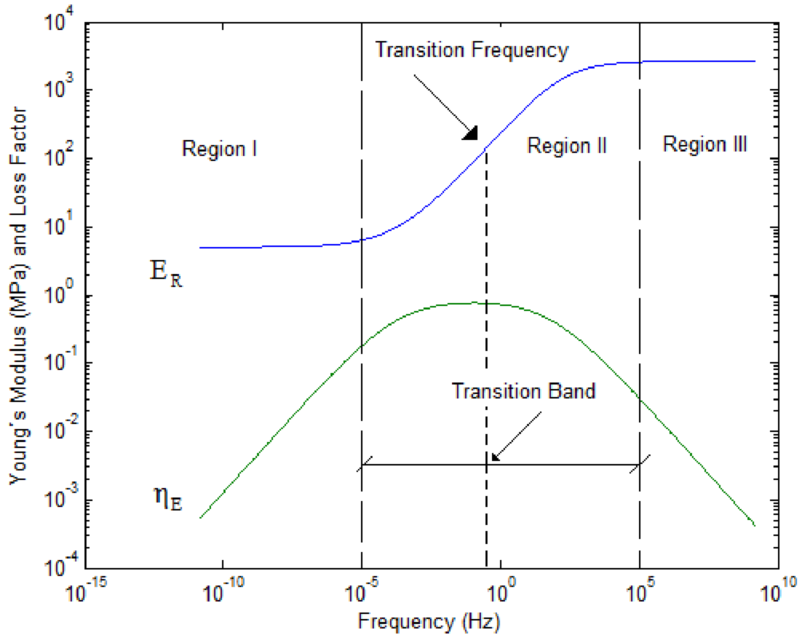

Figure 2 - Variation of E_R e η_E with frequency in a typical viscoelastic material.

2.3 Master Curves

Due to its frequency-temperature dependence, it is possible to express the real modulus, from Eq. (03), as

$$\overline{E}(\omega,T) = E_R(\omega,T)[i + i\eta_E(\omega,T)] \tag{04}$$

where ω represents the frequency in rad/s, and T the temperature.

In order to use information about the real modulus and its corresponding loss factor in usual vibration control action, it is necessary to test the material in wide ranges of frequency and temperature. After testing the material at of concern each temperature in a given frequency range, it is obtained a set of experimental curves. Those curves can be superimposed by the use of the frequency-temperature superposition principle to obtain a complete characterization.

The principle says that, for some materials, the frequency dependence and the temperature dependence can be related to a unique composite variable, which combines the effects of frequency and temperature (Jones, 1989; Ferry et al., 1952). Thus, the distinct experimental curves can be superimposed at a unique reference temperature by appropriate shifts in frequency, giving rise to a single master curve for each dynamic property. Therefore, for the dynamic properties, the following expressions hold

$$E_{R0}(\omega_R) = (T_0\rho_0/T\rho)E_R(\omega,T) \tag{05}$$

$$(\eta_E)_0(\omega_R) = \eta_E(\omega,T) \tag{06}$$

where T_0 is the reference temperature, ρ is the density, ρ_0 is the density at the reference temperature, $\omega_R = \alpha_T(T)\omega$ is the so called reduced frequency, and α_T is the shift factor, whose values are $0 < \alpha_T < 1$ for $T > T_0$, $\alpha_T = 1$ for $T = T_0$ and $\alpha_T > 1$, for $T < T_0$.

The above expressions establish that, except for the factor given by $(T_0\rho_0/T\rho)$ for the real modulus, the dynamic properties in a frequency ω and at a temperature T are equal to the dynamic properties in a composite frequency ω_R, in the reference temperature T_0. Each $\alpha_T(T)$ yields a variation in frequency equivalent to the change in temperature from T to T_0, and thus the variables frequency and temperature are replaced by the single composite variable ω_R, called, then, reduced frequency.

The appropriate description of the shift factor α_T is very important during the characterization. The empirical equation of Williams-Landel-Ferry (WLF) (Williams et al., 1955) and the theoretical Arrhenius equation (Lewis et al., 1989) proved to be appropriate models representing the shift factor. However the Arrhenius equation has the advantage of being simpler in its application (Mead, 1999).

The empirical equation WLF is given by

$$\log_{10}\alpha_T(T) = \frac{-\theta_1(T - T_0)}{\theta_2 + T - T_0} \tag{07}$$

where θ_1 and θ_2 are parameters to be determined for each material.

As the Arrhenius equation, it is given by

$$\log_{10}\alpha_T(T) = T_A\left(\frac{1}{T} - \frac{1}{T_0}\right) \tag{08}$$

where T_A is the so called activation energy, also to be determined for each material.

After consolidating the various experimental curves into two master curves, the dynamic properties can be presented in a plot called reduced frequency nomogram (Jones, 1978; Nashif et al., 1985; Jones, 2001), as illustrated in Fig. 3.

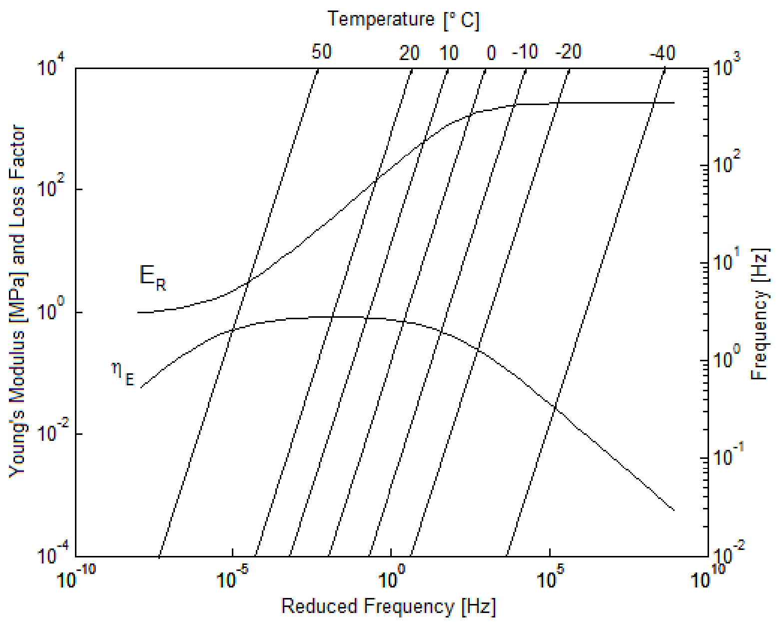

Figure 3 –Reduced frequency nomogram.

3 FRACTIONAL DERIVATIVE MODEL

The fractional derivative models have proved to be efficient in describing the dynamic behavior of various viscoelastic materials, particularly those used in the vibration control (Pritz, 1996). The fractional derivative models, besides describing adequately the behavior of viscoelastic materials, are very convenient for engineering calculus in the frequency domain.

The generalized model of fractional order which gives an one-dimensional constitutive equation for the viscoelastic materials, according to Bagley and Torvik (1986), is

$$\sigma(t)+\sum_{m=1}^{M} b_m D^{\beta_m}\left[\sigma(t)\right]=E_0\varepsilon(t)+\sum_{n=1}^{N} E_n D^{\alpha_n}\left[\varepsilon(t)\right] \tag{09}$$

where b_m, β_m, E_0, E_n and α_n are real parameters, $\sigma(t)$ and $\varepsilon(t)$ are the time histories of stress and strain, and D^{α_n} and D^{β_n} are operators of derivatives of fractional order. By taking m=n=1, $\beta_1=\alpha_1=\beta$ and $b_1=b$ in Eq. (09), and then applying the Fourier transform, it folows a switable model for the complex Young's modulus of a viscoelastic material in the frequency domain, with four material parameters (Bagley and Torvik, 1986). It is

$$\bar{E}(\omega)=\frac{\bar{\sigma}(\omega)}{\bar{\varepsilon}(\omega)}=\frac{E_L+E_H b(i\omega)^{\beta}}{1+b(i\omega)^{\beta}} \tag{10}$$

where E_L is the elastic modulus, E_H is the glassy modulus, b is a real parameter and β is the order of the associated fractional derivative, so that $0<\beta<1$.

As the viscoelastic material also shows a temperature dependence, which is of great importance in vibration control, Eq. (10) can be accordingly written as follows:

$$\bar{E}(\omega,T)=\frac{E_L+E_H b\left[i\alpha_T(T)\omega\right]^{\beta}}{1+b\left[i\alpha_T(T)\omega\right]^{\beta}} \tag{11}$$

Due to the fact that Eq. (11) also includes the shift factor, the shift factor is added, the parameters associated with the chosen equation of that factor have to be taken into account as well, as for as the dynamic characterization of the material is concerned are added. In case of using Eq. (07) two additional parameters should be considered, which gives six parameters to be identified. If Eq. (08) is employed, there is one additional parameter and five parameters to be identified. To ensure the thermodynamics constraints of the model, it follows that $E_H>E_L>0$ and $b>0$, assuming that $0<\beta<1$, (Bagley and Torvik, 1986).

As reported by Medeiros Junior (2010), each of the four parameters in Eq. (10) can be related to specific features of the real modulus and loss factor curves. That author showed this relationship for each one of the parameters by varying the parameter of interest while keeping the others fixed.

It is verified that the parameter E_L gives the lower asymptotic value of the real modulus curve. The greater the E_L value is, the greater the values of the real modulus below the frequency of transition are. As to the parameter E_H, it gives the upper asymptotic value of the real modulus curve. It is also seen that the parameter b is associated with the location of the transition frequency. As to the parameter β, it explains the slope of real modulus curve in the transition region and also the value and location of the loss factor peak. Further details can be found in Medeiros Junior (2010).

4 BAYESIAN MODEL

The Bayesian inference (Migon et al., 2015) quantifies the uncertainty about model parameters within an unknown vector θ in the form of a probability distribution. A prior probability distribution is assigned to each individual parameter, or element, of this vector and combined with the likelihood function for the observed data such that a posterior distribution for each parameter can be obtained. This method is based on the Bayes theorem (Migon et al., 2015), and can be stated as

$$p(\theta \mid y) = \frac{p(\theta, y)}{p(y)} = \frac{p(\theta)p(y \mid \theta)}{p(y)} \tag{12}$$

where $p(\theta \mid y)$ is the posterior distribution, $p(y \mid \theta)$ is the likelihood function, which incorporates the information in the data, and $p(\theta)$ is the so called priori distribution. There is also a normalization factor, $p(y)$, ensures the posterior distribution integrate to one over the domain of θ.

The likelihood function for the model considered here will be obtained assuming that the errors are independent and normally distributed. The function $f(\cdot)$ has as its arguments the temperature, the frequency and the vector theta of unknowns. Thus the model becomes,

$$Y = f(\text{temperature, frequency, } \theta) + \varepsilon \tag{13}$$

where $\varepsilon \sim N(0, \sigma^2)$ and Y is the observable response variable.

The function $f(\cdot)$ represents the model for the Young's modulus and the vector θ consists of $\{E_L, E_H, b_0, \beta, \theta_1, \theta_2\}$, or $\{E_L, E_H, b_0, \beta, T_A\}$ according to the chosen shift factor equation. The elements of θ are the parameters associated to the dynamic properties of a given viscoelastic material.

The prior distributions should be carefully chosen for each parameter according to their domain and meaning in the dynamic characterization process. The characterization should follow the thermodynamic restrictions presented in section 3. The priors were chosen with mean values taken from a previous work presented in Balbino (2012), an a large variance in an attempt to produce weekly informative priors that are likely to produce posteriors which are dominated by the data. Bearing that in mind, the chosen priors herein were

$$E_L \sim \text{Truncated Normal}\left(\mu_{E_L}, \sigma^2_{E_L}\right), E_L \in (a,b), \text{ where } \mu_{E_L} = 5 \text{ e } \sigma^2_{E_L} = 1000000;$$
$$E_H \sim \text{Normal}\left(\mu_{E_H}, \sigma^2_{E_H}\right), \text{ where } \mu_{E_H} = 2395 \text{ e } \sigma^2_{E_H} = 1000000;$$
$$b_0 \sim \text{LogNormal}\left(\mu_{\ln(b_0)}, \sigma^2_{\ln(b_0)}\right), \text{ where } \mu_{\ln(b_0)} = 0{,}004 \text{ e } \sigma^2_{\ln(b_0)} = 1000000;$$
$$\beta \sim \text{Truncated Normal}\left(\mu_\beta, \sigma^2_\beta\right), \beta \in (0,1), \text{ where } \mu_\beta = 0{,}4 \text{ e } \sigma^2_\beta = 1000000;$$
$$\theta_1 \sim \text{Normal}\left(\mu_{\theta_1}, \sigma^2_{\theta_1}\right), \text{ where } \mu_{\theta_1} = 40 \text{ e } \sigma^2_{\theta_1} = 100;$$
$$\theta_2 \sim \text{Normal}\left(\mu_{\theta_2}, \sigma^2_{\theta_2}\right), \text{ where } \mu_{\theta_2} = 300 \text{ e } \sigma^2_{\theta_2} = 100;$$
$$T_A \sim \text{Normal}\left(\mu_{T_A}, \sigma^2_{T_A}\right), \text{ where } \mu_{T_A} = 8000 \text{ e } \sigma^2_{T_A} = 1000000.$$

The posterior distributions are approximated by Markov Chain Monte Carlo (MCMC) (Gilks et al., 1996) simulations using the package RJAGS (Plummer, 2014) for the statistical computing environment R (R Development Core Team, 2015). The MCMC sampling algorithm is higly flexible and able to sample from non-linear and complex models with distributions other than Gaussian for which analytical results and other sampling methods could not be feasible. The method consists of a random walk over the parametric space followed by an acceptance-rejection criterion driven by the likelihood function, which guarantees appropriate results. After certain number of iterations, it is possible to reach the stationary posterior distribution. Through diagnostic plots and other measures, it is possible to check the representativeness, precision and efficiency of the MCMC (Kruschke, 2014).

5 EXPERIMENTAL APPLICATION

The experimental data used in this work was the same reported in Balbino et al. (2013). The dynamic properties were raised with the aid of a specific equipment called NETZSCH DMA 242 C. A typical viscoelastic material, commercially known as ISODAMP C-1002 and manufactured by EAR Specialty Composites, was employed in the tests. A total of 25 sample units were tested. The dimensions of each sample unit were 10 mm long, 4 mm wide and 1.37 mm thick. Previous experiences in the characterization of viscoelastic materials, drawn from Jones (1989, 1992, 2001), Lopes (1998), Lopes et al. (2004) and Espíndola et al. (2003, 2005) allowed the selection of 10 frequencies, namely: 0.1Hz, 0.2Hz, 0.5Hz, 1Hz, 2Hz, 5Hz, 10 Hz, 20 Hz, 50Hz and 100Hz.

The temperatures were also chosen based on previous experiences, on the manufacturer's nomogram and on three preliminary tests of dynamic characterization, performed with the complete experimental set-up. These temperatures, in a total of 7, were the following: -40 °C, -20 °C, -10 °C, 0 °C, 10 °C, 20° C and 50 °C. The smallest interval around 0 °C was due to the fact that the transition region of the material lies within that range. Fig. 4 shows a sample unit in the corresponding clamping device of the equipment, just above its thermal chamber.

Figure 4 – Sample unit of viscoelastic material in the equipment.

6 RESULTS AND DISCUSSION

As stated previously, the concern is to apply the Bayesian approach to carry inference upon the dynamic properties of a viscoelastic material, through a probabilistic model that incorporates the uncertainties from experimental data and model specification.

As a first step to implement the Bayesian inference, a set of prior distributions for the parameters was proposed, as explained in section 4 according to their domain and constraints imposed by the model. The parameter E_L was truncated in the interval $E_L \in (0,10)$. To determine this interval, different ranges and distributions were tested, observing the thermodynamic constraints of the model. The parameter β was truncated in the interval $\beta \in (0,1)$ since it is a restriction of the four-parameter fractional derivative model.

Samples from the posterior distribution of θ were obtained considering a wide variation in frequency and temperature. A total of 10,000 MCMC simulations were performed after a burn-in of 500 iterations, which were regarded as enough to achieve the stationary distribution and, consequently, convergence of the chain. Plots with diagnostics for the chain were generated, showing that the results from the simulations were satisfactory.

Samples from the marginal posterior distributions, obtained via MCMC, are displayed in Fig. 5 and 6. Fig. 5 shows the estimated parameters under the WLF equation for the shift factor while Fig. 6 shows the estimates using the Arrhenius equation.

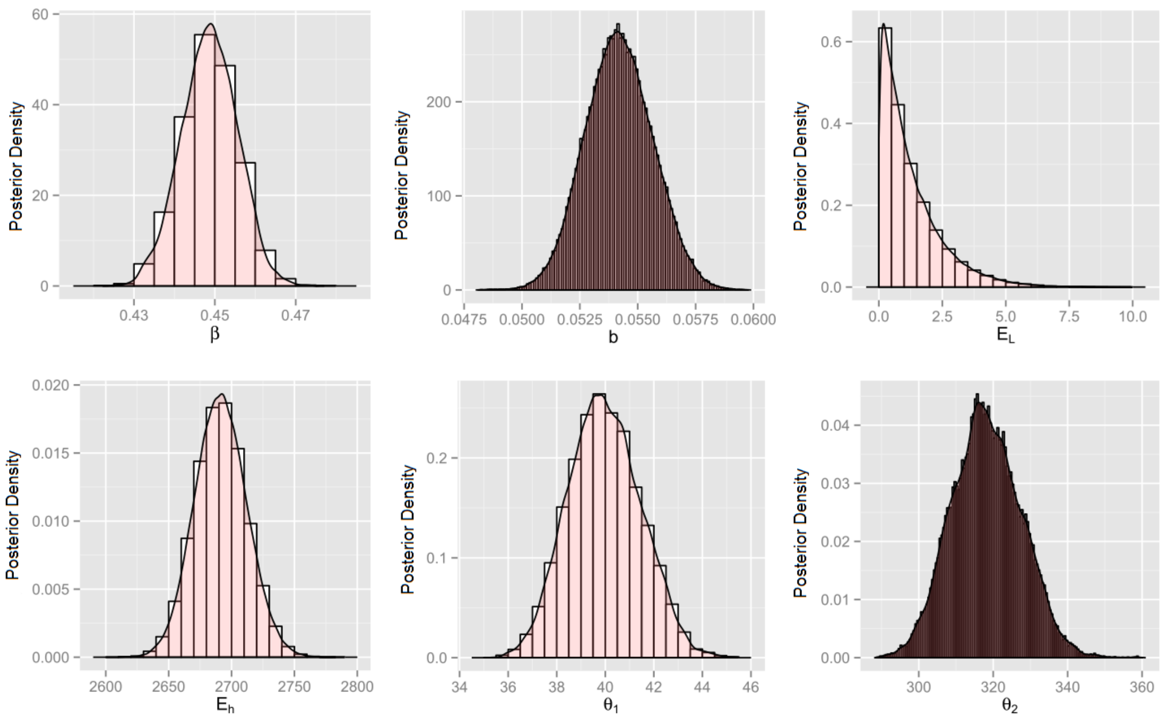

Figure 5 – Posterior probability density functions of the parameters using the WLF equation.

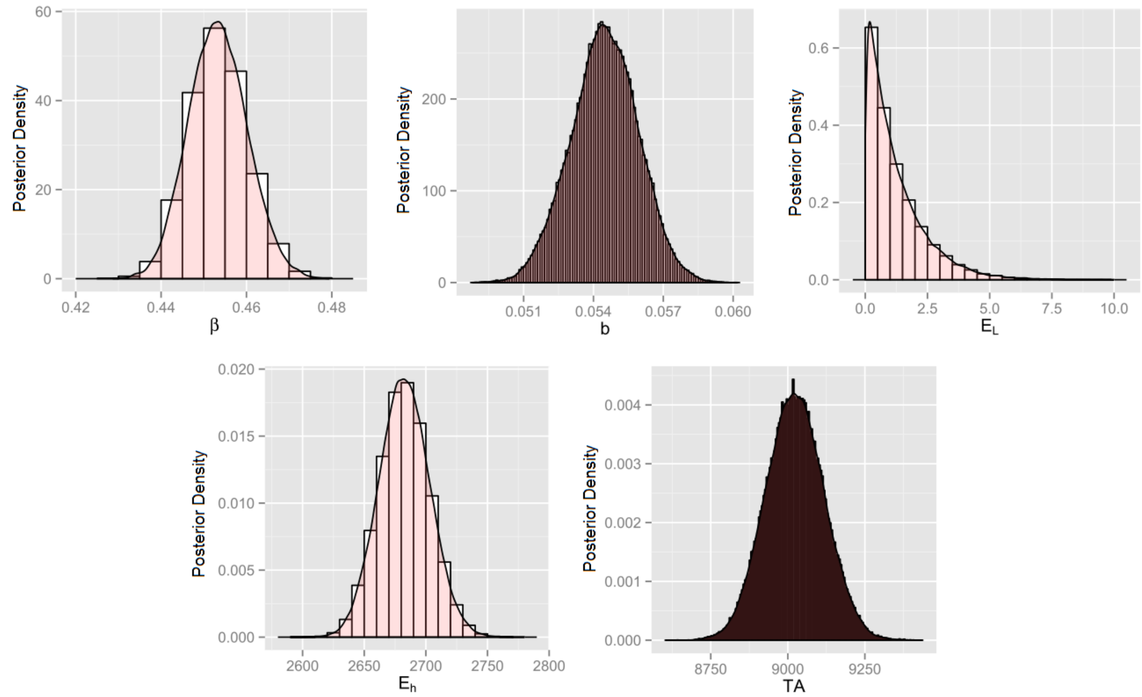

Figure 6 – Posterior probability density functions of the parameters using the Arrhenius equation.

It can be observed in Figs. 5 and 6 that no significant changes occur in the four parameters of the fractional derivative model. That means the two shift factor equations perform similarly in the chosen range of temperature and frequency. However, the Arrhenius equation, which has one parameter less than the WLF equation, has the advantage of being a more parsimonious representation.

It is important emphasize that, for efficacious vibration control actions, the dynamic characterization should be carried out in a broad range of temperatures, since a single temperature experiment can produce misleading results (Espíndola et al., 2003). To illustrate this fact, Fig. 7 displays the Posterior distributions for the parameters when considering only the data at 20°C. In this case, as the temperature is not a variable, it is Eq. (10), of section 3.

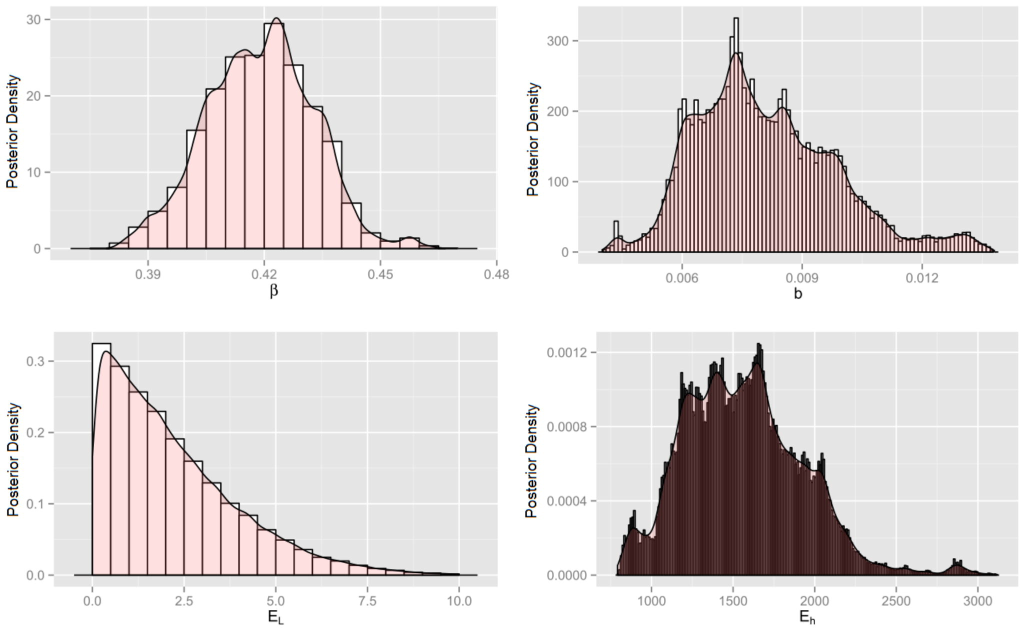

Figure 7 – Posterior distribution density of the parameters at 20°C.

It is noticed in Fig. 7 that the results at 20°C are discrepant from those shown in Figs. 5 and 6, which consider all the temperatures. The parameters E_L, E_H, β and b are not estimated with the same accuracy as it occurs with the complete data set. After running the diagnostics for the representativeness and convergence of the MCMC, they indicate the failure in reaching the target distribution. Some attempts to improve the results, like increasing the length of the burn-in stage, were unsuccessfully made. This analysis demonstrates the importance of characterizing the dynamic properties of viscoelastic materials in a wide range of both frequency and temperature.

The estimated means of the parameters (obtained from the marginal posterior distributions in Figs. 5 and 6) were employed to plot the reduced frequency nomograms shown in Figs. 8 and 9, corresponding to the use of the WLF and Arrhenius equations, respectively.

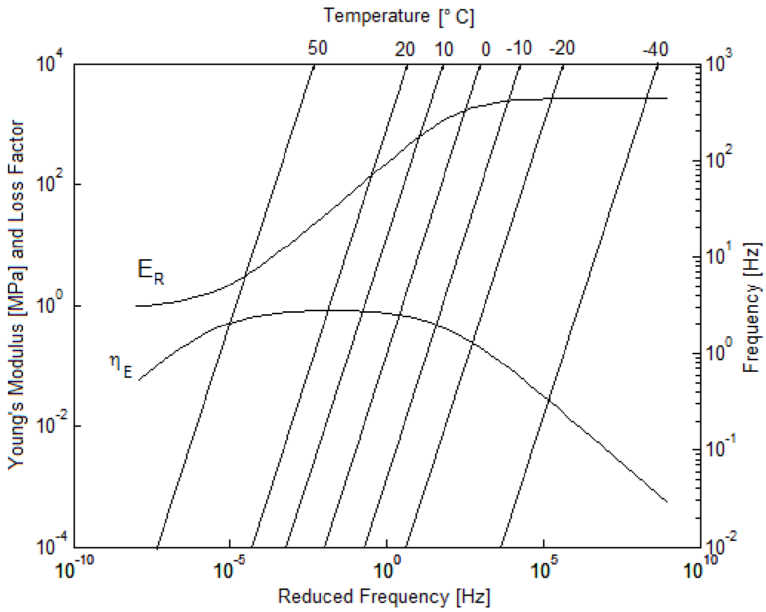

Figure 8 – Reduced frequency nomogram based via estimated means - WLF equation.

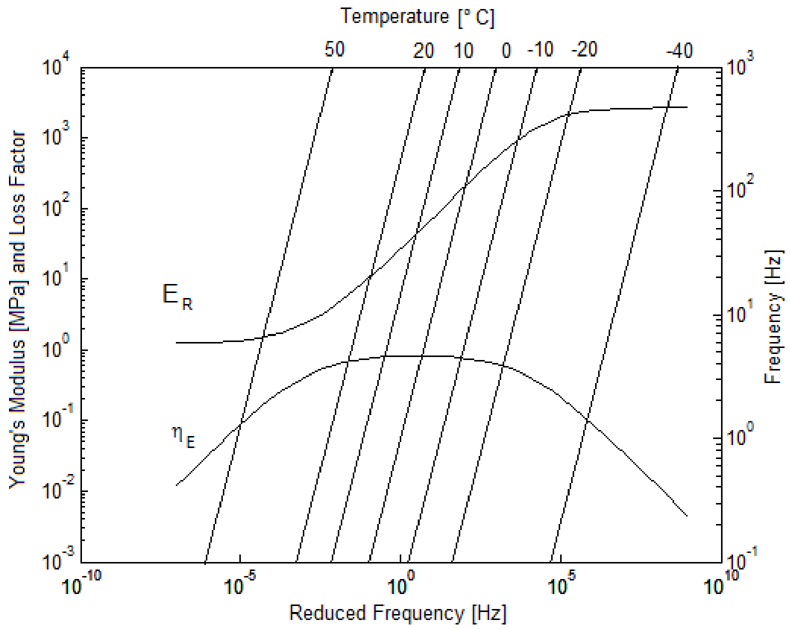

Figure 9 – Reduced frequency nomogram via estimated means - Arrhenius equation.

Both plots are effective in broadly characterizing the dynamic properties of the tested viscoelastic material.

7 CONCLUSION

The Bayesian approach is employed for the dynamic characterization of a typical viscoelastic material in its dependency in frequency and temperature. The representation of the complex Young's modulus is based on the four-parameter fractional derivative model and the WLF and the Arrhenius equations. The Markov Chain Monte Carlo sampler performs the simulations required for the identification of the material parameters. The main advantages of the Bayesian approach in models of this nature, clearly non-linear, is the ability to evaluate more realistically the uncertainties associated with the estimates and curves obtained. It is shown the importance to characterize the dynamic properties of a viscoelastic material in a wide range of frequency and temperature. The Bayesian approach approximates, via MCMC, the posterior distribution for each parameter of the four-parameter fractional derivative model.

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