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Thermorheologically simple materials: A bayesian framework for model calibration and validation

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ABSTRACT

The dynamic properties of viscoelastic materials show highly frequency-temperature dependency and numerical methods for structural systems containing this type of material require accurate mathematical models to describe their dynamical behaviour. The material behaviour here is modelled using a constitutive equation based on fractional derivative operators and considering the temperature dependence of the material under the thermorheologically simple postulate. The quest for information about the constitutive model parameters is phrased as a statistical inverse problem under the Bayesian framework. A Markov Chain Monte Carlo (MCMC) method is used to explore the posterior density of model parameters using measured data from dynamic tests at different temperatures. The agreement between measured data and the predictive capabilities of sixteen models were quantitatively assessed using two validation metrics. Based on the validation metrics analysis it is possible to conclude that the range of temperature of the calibration data set is a key-point into the implementation of the Frequency Temperature Superposition Principle (FTSP). This was verified defining some scenarios for assessing the agreement of model predictions and the set of available experimental data. The results are quite compelling due to the fact that the proposed approach is easy-handed. Furthermore, this approach could be applied on any generic constitutive model using the FTSP.

1. Introduction

The use of constitutive models to describe the dynamical behaviour of Viscoelastic Materials (VEM) has increased in different areas of engineering and applied sciences and the knowledge of their dynamic properties is necessary in order to use them for predictive, risk and optimisation analysis. VEM have complex dynamic characteristics and their dynamic response depends on several environmental variables such as the temperature, frequency range of operation, preload and amplitude as shown by Jrad et al. [1].

The mechanical behaviour of typical viscoelastic materials has strong dependence on temperature [2,3]. The theoretical aspects of constitutive equations for viscoelastic media may be found in the reference books by Christensen [2] and by Drozdov [4]. In particular, there is a specific type of temperature dependence that is amenable to analytical descriptions and which proves useful for modelling a wide range of materials [2]. The materials which presents this type of behaviour are

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defined as being *thermorheologically simple*. The thermorheologically simple postulate is also named as the Time-Temperature Superposition Principle (TTSP) [2] and it has a relation with the Frequency-Temperature Superposition Principle (FTSP). In particular, in order to use the FTSP to obtain a comprehensive representation of the dynamical behaviour of a VEM it is necessary to take into account data sets over some frequency range and at several temperatures.

The FTSP states that there is a mutual correspondence between the frequency and temperature effects, that is, the change in a mechanical property induced by a variation on temperature can be identical to the one produced by a variation on frequency [2,5,6]. In general, the FTSP is used by materials manufacturers or even by most of the laboratories towards generating nomogram representations [7,8]. In other words, it is quite common to use the FTSP to adjust exclusively experimental data in a Master Curve to generate nomograms. These experimental nomograms provide means to obtain information about the material behaviour as a function of temperature and frequency. Their construction demands the use of relatively expensive equipment and frequently (i) requires the prior knowledge of the glass transition temperature T_g, (ii) it does not adjust a constitutive model of the material that involve appropriate thermodynamic constraints according to the dissipative processes involved on the VEM, (iii) it does not allow an uncertainty analysis of the experimental data. Another approach relies on the use of measured data and models. In this sense, some authors have recently approached the VEM characterization task conjugating mechanical models and the FTSP. Moreira et al. in [9] and Madigoski et al. in [6] uses the FTSP and a constitutive model based on fractional derivative operators, Kim and Lee [10], in turn, perform the calibration of a model based on fractional derivative operators using laminated sandwich beams with viscoelastic core. The works in [6,9–11] are based on deterministic inverse analysis and do not present information on data uncertainties or model parameter uncertainties.

The present work proposes the calibration of constitutive models for thermorheologically simple VEM based on a Bayesian framework [12]. The rationale for this choice comes from the fact that: (i) it is common knowledge that measurement noise and the signal acquisition/processing methods can affect the quality of the measurement data and (ii) models are built based on assumptions and approximations that are rarely taken into account along the inverse analyses. Therefore, as items (i) and (ii) have an impact on the calibrated models, a probabilistic framework is more suitable to take into account these kind of uncertainties besides being able to properly deal with them.

Many researchers have successfully used a probabilistic approach in parameter estimation, model verification and uncertainty quantification problems. As for VEM characterization, one may cite that recently Oates et al. [13] and Haario et al. [14] used a Bayesian approach to explore and quantify the uncertainty in a constitutive model of VEM based on the concept of internal state variables and Zhang et al. [15] proposed the calibration of a model using a Bayesian approach using experimental data from the frequency response function of a sandwich beam.

This work is a continuation of the one recently presented by Borges et al. [16] in which an approach to assess viscoelastic constitutive models is presented. The contribution of the present work is to introduce a strategy for model calibration and validation of constitutive models for thermorheologically simple materials that relies on a Bayesian framework. This Bayesian framework naturally deals with data uncertainty and model uncertainties as well; moreover, as the strategy provides stochastic models as its output, information concerning model uncertainties may be naturally linked to Model Validation strategies based on the principles of the Verification and Validation field (V&V) [17–20]. In particular, the model assessments and the evaluation of their predictive capabilities are performed with the aid of the dimensionless area validation metric [16] and with a specific metric that takes the entire frequency range of interest into account.

In the following sections, the mathematical formulation for the FTSP and the VEM model formulation based on fractional derivative operators with five parameters is first described, and it is followed by an inverse problem methodology based on a Bayesian approach and the model validation framework. The experimental Set-up was specifically designed for this purpose in which material shear complex modulus can be measured for some temperatures of interest. The analyses of the model parameters as well as the validation metrics is presented and discussed, followed by concluding remarks.

2. Mechanical modeling

The dynamic behaviour of a VEM depends on temperature, frequency and ageing effects [4,21]. As for the modelling of the VEM, this process must be accomplished guided by the information concerning both the operational and environmental conditions at which the VEM will be working. For example, there are a number of applications for which temperature does not play an important role. For these situations, it is quite common to use standard viscoelastic models that are properly calibrated for the specific temperature of interest. In other words, the model is built assuming that the VEM will be working approximately under isothermal mechanical processes. On the other hand, there are several situations for which one cannot neglect temperature effects when building the model for the VEM. For example, models used to provide predictions for components made of polymeric materials that will work outdoors in a region for which there are great temperature variations along the year. For these conditions, modelling do need to take the temperature dependence into account. The model used in this work to describe the behaviour of VEM and the way temperature effects are taken into account are presented next.

2.1. Constitutive model formulation

The constitutive equations for viscoelastic materials can be formulated using hereditary integrals [2,21], internal variables [16,22], mechanical analogs [21] and the complex modulus approach [21]. Under the hypotheses of small