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Research Article

GENETIC ALGORITHM OPTIMIZATION METHOD FOR PARAMETER ESTIMATION IN THE MODELING OF STORAGE MODULUS OF THERMOPLASTICS

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ABSTRACT

Polymeric materials exhibit temperature and rate dependent behavior. Therefore, in the modeling of polymeric and polymer based composite materials, the mechanical properties should be defined as rate and temperature dependent to be able to capture the behaviors. Dynamic mechanical analysis (DMA) is mostly used method to determine the viscous and elastic properties via loss and storage modulus. The storage modulus obtained from DMA and the elasticity moduli relate to the same physical phenomena. Even though the magnitudes of elasticity modulus and the storage modulus are not the same, the variation of modulus values with varying temperature follows the same trend. Therefore in the modeling of polymeric material behaviors, temperature and rate dependent elasticity modulus can be determined using DMA results. The objective of this work is to model the storage modulus which can be used as the elasticity modulus with a proper shift in the material models. For that purpose, a semi crystalline Polypropylene (PP) and amorphous plasticized Polyvinyl Chloride (PPVC) thermoplastics are selected to show the applicability of the model for amorphous and semi crystalline polymers. Different from many works in the literature, Genetic algorithm (GA) optimization method is used for parameter estimation in the modeling of storage modulus of PPVC and PP. The parameter optimization procedure is successfully implemented for the case of two polymers. The experimental storage modulus versus temperature curves of PP and PPVC obtained from [1, 2] respectively are used for validation. Good match with experimental data is observed. The rubbery state and rubbery flow observed in semi crystalline PP and sudden drop in the modulus around the glass transition temperature seen in amorphous PPVC are successfully simulated.
Keywords: Storage modulus, polymer, genetic algorithm, modeling.

1. INTRODUCTION

Polymeric materials and polymer-based composites are widely used in engineering applications such as automotive and aerospace industries where wide range of temperatures are involved. The usage of thermoplastics has been increased over the years due to properties such as low cost, low density, corrosion resistance.

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Polyvin yl Chloride (PVC) is one of the most commonly used thermoplastic polymers. The properties of PVC can be enhanced by compounding PVC with a number of additives such as plasticizers, heat stabilizers, and lubricants. PVC used in the automotive industry is generally modified by plasticizing to obtain flexible one. This is called plasticized PVC (PPVC). Plasticizers are generally low molecular weight organic additives which are used to soften rigid polymers, [2]. On the other hand, Polypropylene (PP) has been widely used in composite fabrication because of its good balance between properties and cost as well as its easy processability and low density. PP is generally modified with nanoparticles to fabricate high performance PP engineering plastics. It has been used as matrix material for nanocomposites. Nanoparticles, such as carbon nanotubes (CNTs), graphene, clay are used as filler to produce nanocomposites with desired properties [3, 4]. These two materials, PP and PPVC are selected to model the storage modulus determined from dynamic mechanical analysis (DMA). Measuring both elastic and viscous properties are possible with this method. Glass transition temperature and other transitions will be also determined. Therefore, in the characterization of polymers, it has been used extensively.

In the work by Colak and Acar [5], it is shown that there is a correlation between the storage modulus obtained from DMA and the elasticity modulus obtained from stress-strain curve. The storage modulus is related to the elastic contribution of the total viscoelastic behavior. The elasticity modulus is defined as resistance to elastic deformation and obtained from the slope of the stress–strain curve in the elastic region. Therefore, these two moduli definitions relate to the same physical phenomena which is elastic deformation. Even though the magnitudes of elasticity modulus and the storage modulus are not the same, the variation of modulus values with varying temperature follows the same trend. Due to this finding, the storage modulus has been recently used in the material modeling [1, 2, 5, 6].

Wang et al. [1] investigated the elastic behavior of PP and PP based organoclay nanocomposites. Both DMA and high strain rate uniaxial compression tests (split Hopkinson pressure bar) were used to investigate the elastic behavior of the materials. Richeton's statistical model [6] was used to describe the dependence on temperature and strain rate/frequency of the stiffness of pure PP. The predictions for both storage modulus and compressive modulus for pure PP showed a good agreement with the experimental data. The mechanical behavior of a plasticized poly(vinyl chloride) manufactured through a multilayered process for the automotive industry is investigated by Bernard et al. [2]. The evolution of the storage modulus from the glassy region to the rubbery region is modeled.

To describe the finite mechanical response of amorphous polymers over a wide range of temperatures and strain rates, including the rubbery region and for impact loading rates, a robust physically consistent three-dimensional constitutive model is developed by Richeton et al. [6]. For a wide range of temperatures and strain rates, the simulated results for poly(methyl methacrylate) (PMMA) and polycarbonate (PC) are depicted and it is shown that they are in good agreement with experimental observations.

Optimization methods have been widely used in different fields in order to solve the problem of parameter estimation [7, 8, 9]. In the work by Guo et al. [9], a hybrid GA-BFGS algorithm is introduced to determine the parameters in the ADF model. BFGS algorithm is introduced into a GA framework as a basic operator in order to reduce the iteration times as possible. The material parameters of VBO model are determined using uniaxial loading–unloading stress strain curves of high density polyethylene (HDPE). Using these material parameters, creep and relaxation behaviors of HDPE are simulated, [10]. The numerical modeling of the mechanical behavior of anisotropic concrete damage model is performed by Wardeh and Toutanji [8]. A Genetic algorithm FORTRAN subroutine is used to estimate the parameters based on the coupling between the constitutive and damage evolution equations.

Literature review reveals that the storage modulus has been used in the material modeling. However, the material parameters in the modulus formulation are determined using trial and error analysis [1, 2, 5, 6]. Any optimization methods for material parameter estimation is not used in these works. Different from the most of the works in the literature, GA is used in the parameter estimations of the frequency and temperature dependent storage modulus formulation which consist of 13 parameters. To show the modeling capabilities, both amorphous and semi-crystalline polymer are selected. For temperature and frequency dependent behavior of semi-crystalline PP and amorphous PPVC thermoplastics, the storage modulus defined considering β, α (glass transition) transitions and flow by [6] is used. Simulation results are compared to experimental data by Wang et al. [1] and Bernard et al. [2]. Good match between simulations and experimental results are obtained.

2. MATERIAL PARAMETER DETERMINATION WITH GENETIC ALGORITHM OPTIMIZATION METHOD

GA is based on a natural selection process that mimics biological evolution. GA starts with chosen an arbitrarily population of individuals. The algorithm repeatedly modifies a population of individual solutions. The optimization procedure searches for the best individual by considering the fitness function in the population. At each step, the genetic algorithm randomly selects individuals from the current population and uses them as parents to produce the children for the next generation. These individuals, called elite are passed to the next population [11, 12].

The fitness function used in the optimization was,

$$F(\boldsymbol{x}) = \sum_{i=1}^{N} \left| \sigma_i^{exp} - \sigma_i^{sim}(\boldsymbol{x}) \right| \tag{1}$$

where N is the number of measurement points, x={} is a vector of model parameters, σ_i^{exp} is experimentally obtained stress and $\sigma_i^{sim}(x)$ is stress obtained by the simulation.

In this work, the experimental storage modulus versus temperature curves of PC and PPVC obtained from Wang et al. [1], Bernard et al. [2] respectively are used. The fitness function includes the differences between experimentally determined and the simulated results of storage modulus for one frequency.

GA optimization procedure was implemented by using MATLAB. The programs consist of GA optimization M-File for obtaining parameters and IMS Fortran scripts of the model. In order to determine material parameters of the model, MATLAB scripts and IMLS FORTRAN script are used repeatedly. Fitness values versus generation during the model parameter optimization for PP and PPVC are depicted in Fig. 1 and 2 respectively.

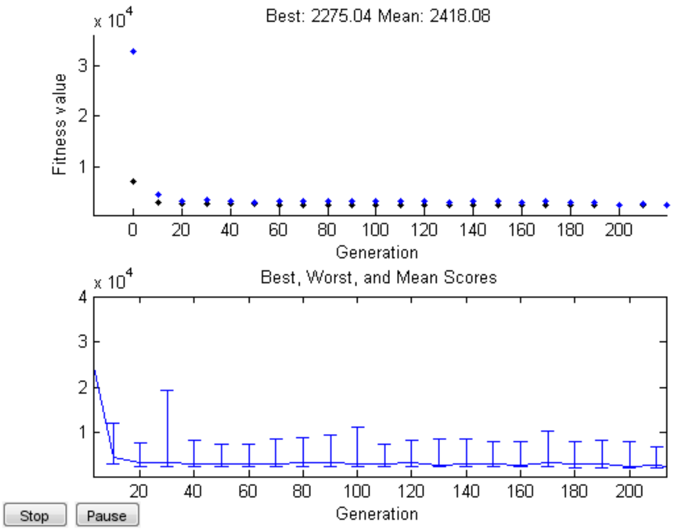

Figure 1. Fitness values versus generation during material parameters optimization of PP

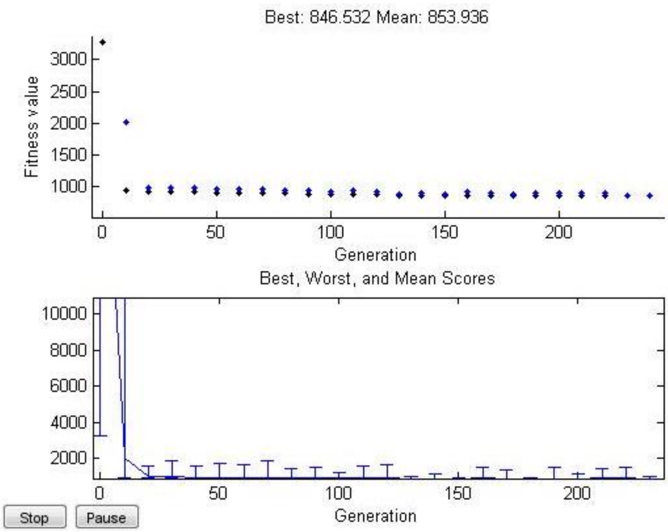

Figure 2. Fitness values versus generation during material parameters optimization of PPVC

3. DYNAMIC MECHANICAL ANALYSIS (DMA)

DMA has been used extensively since measuring both elastic and viscous properties is possible with this method. By applying an oscillatory strain to a polymer sample, resulting sinusoidal stress is measured. The strain input is given by

$$\varepsilon(t) = \varepsilon_o \sin(\omega t) \tag{2}$$

The associated stress will respond with the same frequency but with a phase difference,

$$\sigma(t) = \sigma_o \sin(\omega t + \delta) = E(\omega)\varepsilon_o \sin(\omega t + \delta) \tag{3}$$

Where δ is the phase angle which describes the viscous character of the material. For viscoelastic materials, the phase angle is between 0 and π/2. $E(\omega)$ is the dyanamic modulus defined by the ratio of stress to strain ($E(\omega) = \sigma_o/\varepsilon_o$)

An alternative representation of stress is defined as

$$\sigma(t) = E'(\omega)\varepsilon_o \sin(\omega t) + E''(\omega)\varepsilon_o \cos(\omega t) \tag{4}$$

Where $E''(\omega)$ is the storage modulus, $E'(\omega)$ is the loss modulus. It describes the viscous part of the stress response.

Storage and loss modulus of the material is determined with respect to temperature. DMA is used to determine the glass transition temperature of the material. When the test is performed for a given range of temperature, the modulus values exhibit changes at three temperature values which are called transition temperatures. Those transitions are entitled to secondary relaxation, glass transition, and flow (T_β, T_g, T_f). It is considered that temperature transitions requires breakage of secondary chemical bonds.

4. MODELING TEMPERATURE AND STRAIN RATE DEPENDENT STORAGE MODULUS

For modeling temperature and rate dependent behavior of polymers, the storage modulus is defined considering β, α (glass transition) transitions and flow, [6] as given in Eq. 5.

$$E(\theta, f) = (E_1(f) - E_2(f))\exp\left[\left(-\frac{\theta}{T_\beta(f)}\right)^{m_1}\right] \tag{5}$$
$$+(E_2(f) - E_3(f))\exp\left[\left(-\frac{\theta}{T_g(f)}\right)^{m_2}\right] + E_3(f)\exp\left[\left(-\frac{\theta}{T_f(f)}\right)^{m_3}\right]$$

where $E_i(f)$ is only frequency dependent. It is the stiffness of the material at the beginning of each transition i. m_i are the Weibull moduli corresponding to the statistics of bond breakage and the transition temperatures T_β, T_α and T_f. The transition temperatures are found by dynamic mechanical analysis (DMA). The instantaneous stiffness is given as,

$$E_i = E_i^{ref}\left(1 + s\, log\left(\frac{f}{f^{ref}}\right)\right) \tag{6}$$

where s is a material constant representing the sensitivity of the modulus to frequency (or strain rate). In the determination of $T_\beta(f)$, secondary relaxation temperature at the frequency f, the β movements are activated by an Arrhenius process. It is given as

$$\frac{1}{T_\beta} = \frac{1}{T_\beta^{ref}} + \frac{R}{\Delta H_\beta} ln\left(\frac{f^{ref}}{f}\right) \tag{7}$$

Where T_β^{ref} reference β relaxation temperature, ΔH_β is the β activation energy, R is the Boltzmann constant. The glass transition is described by the free-volume theory and a phenomenological dependence can be used to depict the rate dependence of the flow temperature T_f. [6, 13]

$$T_g = T_g^{ref} + \frac{-c_2^g log\left(\frac{f^{ref}}{f}\right)}{c_1^g + log\left(\frac{f^{ref}}{f}\right)} \tag{8}$$

Where c_1^g and c_2^g are WLF parameters relative to Tg. The flow temperature at frequency f is defined as Eq. 9, [6]

$$T_f = T_f^{ref}\left[1 + 0.01 log\left(\frac{f}{f^{ref}}\right)\right] \tag{9}$$

At a chosen reference frequency, $(f), E_i^{ref}, T_\beta^{ref}, T_g^{ref}$ and T_f^{ref} are the instantaneous stiffness, and temperatures at three main transition respectively.

5. SIMULATION RESULTS

The experimental results of the dynamic mechanical analysis of PP performed by Wang et al. [1] is used for validation of the model. Wang et al. [1] performed DMA tests at various frenquencies (1 Hz and 10 Hz), a constant load of 0.5 N and a temperature range from -80 to 120 ^oC. The material parameters are determined using GA at 1 Hz frequency. The storage modulus versus temperature curve at a frequency of 1 and 10 Hz for PP are depicted in Fig. 3a and b. As seen, it is successfully modeled for both above and below the glass transition regions. The material parameters of storage modulus determined using GA optimization algorithm is given in Table 1.

Table 1. Material parameters of obtained by GA for modeling the storage modulus for PP and PPVC

Parameters	**PP**	**PPVC**	**Unit**
$E_1^{ref}, E_2^{ref}, E_3^{ref}$	4658.89, 4000.05, 720.02	3005.16, 2894.36, 694.91	MPa
T_β^{ref}, T_g^{ref}, T_f^{ref}	150.02, 200, 425.2	-44.35, -37.25, -24.95	C
c_1^g, c_2^g	22.77, 37.48	23.63, 54.99	-, C
m_1, m_2, m_3, s	1.6, 3.59, 18.87, 0.024	4.67, 14, 22, 0.022	-

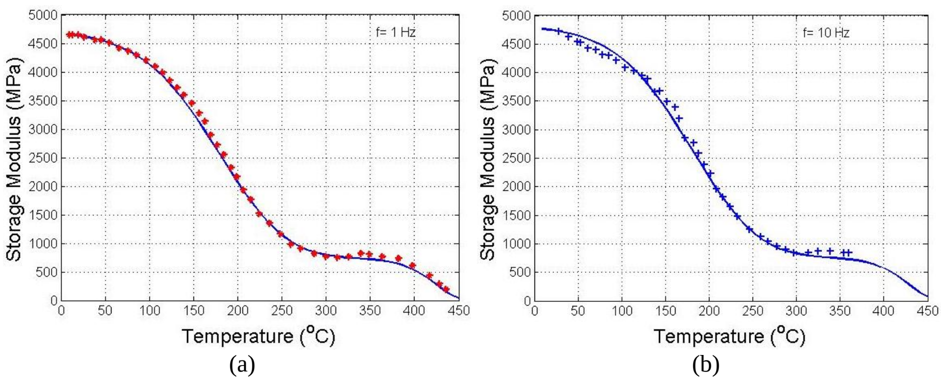

Figure 3. Modeling storage modulus of PP and comparison with the experimental data from Wang et al. [1], a. 1 Hz, b. 10 Hz

PP shows a definite rubbery state and rubbery flow. Glass transition temperature of PP is around -20 °C, - 10 °C region. Increase in frequency leads to an increase in storage modulus. Good agreement with experimental data is obtained.

DMA of PPVC performed at 1 Hz frequency for temperature ranging from -100 °C to 120 °C is modeled in the next simulations. The modeling results for the storage modulus of PPVC at 1 Hz is given in Fig. 4. Apart from the behavior of PP, rubbery state is not observed in PPVC. The glass transition temperature is around -40 °C. Sudden drop in the modulus is seen. As seen from Fig. 4, simulation result match well with experimental data.

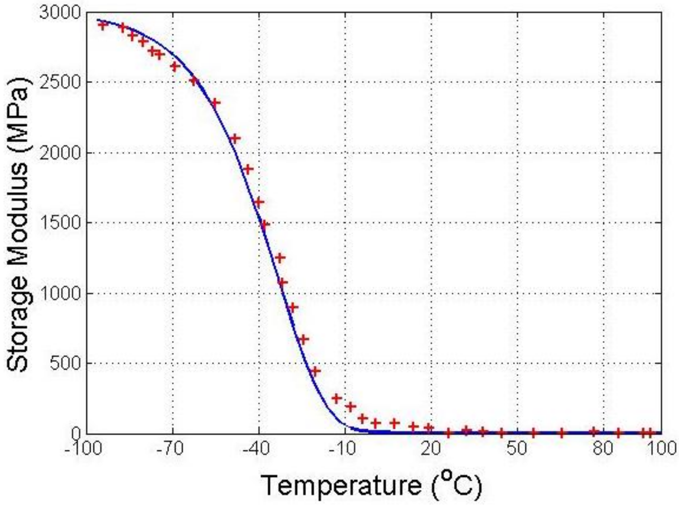

Figure 4. Modeling storage modulus versus temperature curve of PPVC and comparison with the experimental data from Bernard et al. [2]

6. CONCLUSIONS

Due to the correlation between the storage modulus obtained from DMA and the elasticity modulus obtained from the conventional tensile or compression tests [5], the storage modulus has been used extensively in the modeling of material behaviors. In this work, the aim was to determine the material parameters of the storage modulus equation used by Richeton et al. [6] using a genetic algorithm optimization method. Since the material parameters determination is generally made by trial and error analysis in the literature, this work mainly differs with this aspect. On the other hand, both semicrystalline and amorphous polymers are considered. This procedure is verified for the case of two thermoplastic polymers, semicrystalline PP and amorphous PPVC.

Temperature and frequency dependent storage modulus of PP at 1 and 10 Hz and PPVC at 1 Hz frequency are modeled. The simulation results are compared to the experimental data from Wang et al. [1] and Bernard et al. [2]. Modeling capabilities of the model proposed by [6] have been shown. The reported results (Fig. 3 and 4) prove that the parameter optimization procedure is successfully implemented for the case of two polymers.

Comparing the behaviors of semicrystalline PP and amorphous PPVC reveals that the change of the storage modulus with temperature is quite different. While semicrystalline PP exhibits definite rubbery state and rubbery flow, in amorphous PPVC, rubbery state is not observed. Sudden drop in the modulus is seen. The simulation results reveal that these two types of behavior can be successfully simulated with the used model.

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