OPTIMIZATION PROBLEMS IN NONLINEAR MODELING FOR VISCOELASTIC COMPOSITES

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Abstract

Three types of polymer based materials with different modifications of carbon nano fillers were tested in experimental program on creep at various loading level and on quasistatic loading. The creep data is used to develop a model to describe the relationship between time, stress and strain. To this end, Volterra's equation of second type is employed with Rabotnov's kernel.

With the use of the Rabotnov's kernel comes the need to obtain material-dependent parameters associated with the kernel. The standard least squares approach for parameter estimation requires expensive and error-prone function evaluations. However, the Laplace-Carson transform of the Volterra equation with Rabotnov's kernel has a simple and elegant form. This allows for the development of a methodology for obtaining optimal parameter estimates referred to as Laplace-Carson optimization. The obtained material-dependent parameter estimates based on this approach are shown to fit experimental data well. Questions of sensitivity analysis associated with Laplace-Carson optimization are introduced and scoped for future work.

1 Introduction

Materials having the viscoelastic property respond to stress in such a manner that stress applied in the past affects strain in the present time t. The introduction of time dependence or memory effect leads to the analysis of Volterra's equation of second type [1-2] to model the relationship between stress as a functional of strain

$$\varphi(\varepsilon(t)) = M(t) \tag{1}$$

where $\varphi(\varepsilon(t))$ is a response functional of ε (the so-called instantaneous loading diagram) and $M(t)$ models the material stress resulting from the memory effect and is taken to have form

$$M(t) := \sigma(t) + \int_0^t K(t-\tau)\sigma(\tau)d\tau \tag{2}$$

In practice, equation (1) describes the relations between time, stress and strain successfully for a wide range of materials such as polymers, metals, and composites [2-4].

The most suitable kernel *K(t)* is based on the exponential of arbitrary order function [2] taking the form

$$K(t) := \lambda \sum_{n=0}^{\infty} \frac{(-\beta)^n t^{n(1-\alpha)}}{\Gamma[(1-\alpha)(n+1)]} \tag{3}$$

The exponential of arbitrary order operators combine several important features [2,5].

1) The initial moment singularity at $t = 0$ is integratable.
2) The asymptotic exponential behavior with $t \to \infty$.
3) The resolvent operator is the same type of exponential of arbitrary order with different set of defining parameters.

Using the kernel given in (3) together with the assumption that $\sigma(t) := \sigma$ is a fixed known constant, the integral of (2) can be evaluated, and so (2) becomes

$$M(t) := \sigma\left[1 + \lambda \sum_{n=0}^{\infty} \frac{(-\beta)^n t^{(1-\alpha)(n+1)}}{\Gamma[(1-\alpha)(n+1)+1]}\right] \tag{4}$$

In order to use model (4), material-specific kernel parameter values P = $\{\lambda, \alpha, \beta\}$ are required that lead as closely as possible to the realization of equation (1). The parameter α is determined *a priori* [4]. Thus, only β and λ need to be treated as unknown values that need to be determined through optimization techniques. To underscore the dependence of $M(t)$ on the values of β and λ, the model $M(t)$ is now denoted as $M_{\beta,\lambda}(t)$.

The parameters P = $\{\lambda, \alpha, \beta\}$ associated with (4) are material specific and so need to be estimated for each material. This is usually accomplished with the formulation of a least squares problem whose optimal solutions correspond to the parameter estimates that minimize least square deviation of model (4) against experimental strain observations. Due to the expensive and error-prone nature of evaluating a model of form (4), this work presents a means of obtaining parameter estimates by formulating a linear least squares problem constructed from the Laplace transform of equation (1). This approach is demonstrated on nine data sets corresponding to three materials each tested over three different loading levels. The experimental strain observations are taken for the materials:

1) Pure polyamide polymer (PA),
2) Polyamide polymer with carbon nano fillers (PA+UDD), and
3) Polyamide polymer with ultradispersed diamonds (PA+CNT).

Details on the experimental program are given in [6]. For each of the three materials, creep testing was performed at 30%, 40%, and 50% of ultimate stress level. Using the experimental creep observations, the experimentally determined value of α, and estimates of $\varphi(\varepsilon(t))$ also obtained through experiment, optimal parameter estimates for unknown parameters β and λ are to be determined for each data set.

2 Obtaining Optimal Parameter Estimates with the Application of the Laplace-Carson Transform (LCT)

The optimal parameter estimates that most closely enforce equation (1) are normally obtained using standard nonlinear optimization techniques [7-8] for least squares problems. The least square formulation is given by

$$\min_{\beta,\lambda} \sum_{i=1}^{N} \left(\frac{M_{\beta,\lambda}(t) - \varphi(\varepsilon_i)}{\varphi(\varepsilon_i)} \right)^2$$

where ε_i denotes the experimental strain data. It was shown in [9] that difficulties arising from approximating the value of the infinite sum of $M_{\beta,\lambda}(t)$ include the computational expensiveness, determining where to truncate the sum and avoiding the potential for catastrophic cancellation. To address these issues, a linear least squares problem is formulated by applying the Laplace-Carson transform to both sides of equation (1).

The values $\varphi(\varepsilon_i)$ may be fit with interpolating function $I(t)$. When $I(t)$ is substituted for $\varphi(\varepsilon_i)$, equation (1) becomes

$$I(t) = M_{\beta,\lambda}(t) \tag{5}$$

Let $L\{\cdot\}$ denote the operation of taking the Laplace transform. Then $LI(s) := s{\cdot}L\{I(t)\}$ is the LCT of $I(t)$ and $LM_{\beta,\lambda}(s) := s{\cdot}L\{M_{\beta,\lambda}(t)\} = \sigma\left[1+\frac{\lambda}{s^{1-\alpha}+\beta}\right]$ is the LCT of $M_{\beta,\lambda}(t)$.

Apply the Laplace-Carson transform to both sides of equation (5) to obtain

$$LI(s) = LM_{\beta,\lambda}(s) \qquad \text{for } \operatorname{Re}(s) > 0. \tag{6}$$

The LCT variable s is taken from the set of complex numbers for which $Re(s) > 0$. Define this set $H := \{s \in C \mid Re(s) > 0\}$ as the domain over which $LM_{\beta,\lambda}(s)$ is defined. The following facts taken from the theory of complex analysis [10] justify the use of equation (6) to get optimal parameter estimates.

1. The transforms $LM_{\beta,\lambda}(s)$ and $LI(s)$ define analytic complex functions over $s \in H$.
2. An analytic function is uniquely determined by its output values on an open subset $S \subset H$, or over a line extending infinitely in both directions contained in H (i.e., a vertical line).
3. An inverse to $LM_{\beta,\lambda}(s)$ exists, and, for current purposes (see discussion preceding Theorem 7 of Section 64 from [10] for more details), this is given uniquely by $L^{-1}\{LM_{\beta,\lambda}(s)\} = M_{\beta,\lambda}(t)$.

From these three facts, it follows that if equation (6) can be satisfied over some open subset $S \subset H$ for a given choice of β and λ, then the uniqueness of the inverse transforms would give a corresponding satisfaction of equation (5) in the t domain.

To enforce consistency of equation (6) over an open subset $S \subset H$, we enforce the equations

$$LI(s_i) = LM_{\beta,\lambda}(s_i), \qquad \text{for all } s_i \in S. \tag{7}$$

as closely as possible with an optimal choice of β and λ. In practice, equations of form (7) are considered only for some finite sample $S_N \subset S$ of N values $s_i \in S_N$. Once $S_N \subset S$ is determined, the following least squares problem in the s domain is given.

$$\min_{\beta,\lambda} \sum_{s_i \in S_N} \left(LI(s_i) - LM_{\beta,\lambda}(s_i)\right)^2 \tag{8}$$

The open subset $S \subset H$ should be chosen so that $LI(s)$ and $LM_{\beta,\lambda}(s)$ can be easily and reliably computed for each $s_i \in S_N \subset S$. The least squares problem (8) can be formulated as a linear least squares problem when the decision variables are β and λ. This allows for easy computation of the optimal parameter values β and λ.

3. Results of Numerical Procedures for Optimal Parameter Estimates

In order to formulate optimization problem (8) for each data set, the following need to be determined.

1. An interpolating function $I(t)$.
2. An open region $S \subset H$ and a finite sample set $S_N \subset S$ to suitably approximate $S \subset H$.

Regression Functions: In the past, power regressions have been used for the interpolating function $I(t)$ [9]. In this work, regressions functions having form

$$I(t) = \sum_i c_i \cdot t^{a_i} + \sum_j c_j \cdot e^{-a_j}$$

are found to fit experimental creep data better while having a readily available closed-form LCT. The values $a_i \in (0,1)$, $a_j \in (0,1)$ are fixed, finite in number, and customized for each data set. Once a_i and a_j are fixed, the coefficients c_i, c_j are determined using standard techniques of linear regression. The interpolating functions $I(t)$ are given for each data set in Sections 3.1-3.3.

Sample Regions: The sampled regions $S_N \subset S \subset H$ that tend to yield the best parameter estimates from (8) are those regions that are non-elongated such as squares, hexagons, and circles. (Lines, or highly elongated shapes do not work as well). The sample region used for (8) in this work is an open hexagonal region approximated by the values $s_i \in S_N \subset S$ that are spaced according to a triangular lattice as depicted in Figure 1.

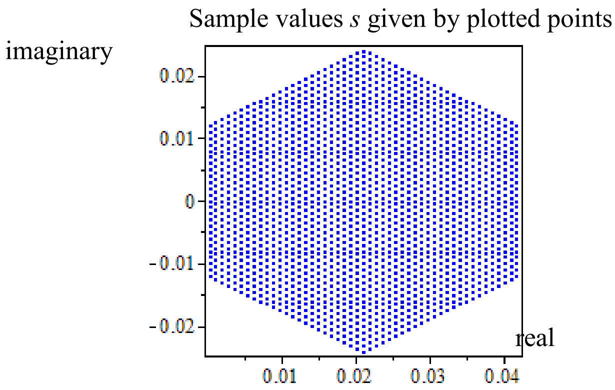

Figure 1. Sample region $S_N \subset S$. The individual $s_i \in S_N$ are depicted with the dots

Subsections 3.1, 3.2, and 3.3 give problem setup information and parameter estimate results for the three materials. For each material, problem setup information refers to the following:

1) The same sample region S_N depicted in Fig.1 is used for every data set.
2) The experimentally determined value of α is stated for each material.
3) The loading level values $\sigma_{0.3}$, $\sigma_{0.4}$ and $\sigma_{0.5}$ are stated for each material.
4) For each material, the function $\varphi(\varepsilon)$ takes linear form $\varphi(\varepsilon) := E\varepsilon$, and the value E is stated.
5) Interpolating function $I(t)$ is stated for each data set.

Once the necessary problem setup information is available, the linear least square solution for each material and loading level specific manifestation of (8) is obtained using the Maple 14 routine LinearAlgebra[LeastSquares] via QR decomposition. These values are given in the results that follow. Lastly, plots are shown giving a comparison of the experimental data, the interpolating function, and the model $M_{\beta,\lambda}(t)$ resulting from the optimal parameter estimates.

3.1. Pure Polyamide (PA)

The non-decision parameter values associated with pure polyamide (PA) are as follows. The parameter α is estimated as α = 0.83. The parameter E associated with the functional $\varphi(\varepsilon) := E\varepsilon$ is determined as E = 955. The loading levels are defined as $\sigma_{0.3}$ = 16.20, $\sigma_{0.4}$ = 21.60, and $\sigma_{0.5}$ = 27.00.

Table 1 gives the interpolating functions $I(t)$ associated with each data set, and also the optimal parameter estimates obtained. Fig. 2 gives plots depicting wellness of fit for model $M_{\beta,\lambda}(t)$ with the experimental and interpolated data.

	Interpolating Functions	Optimal Parameter Estimates	
Loading Level	$I(t) =$	β	λ
$\sigma_{0.3}$	$36.03955\ t^{0.1} - 30.81646\ t^{0.0667} + 6.13278\ t^{0.05}$	0.07665	672.94332
$\sigma_{0.4}$	$2.47000\ t^{0.2} + 31.31428\ t^{0.1} - 19.69854\ t^{0.05}$	0.01945	605.73805
$\sigma_{0.5}$	$9.47225\ t^{0.2} + 19.43801\ t^{0.1} - 11.84635\ t^{0.05}$	-0.02715	556.69281

Table 1. Interpolating functions and optimal parameter estimates for pure polyamide (PA)

Wellness of fit for pure polyamide PA using LCT to obtain optimal parameters β and λ
model   interpolated data   experimental data

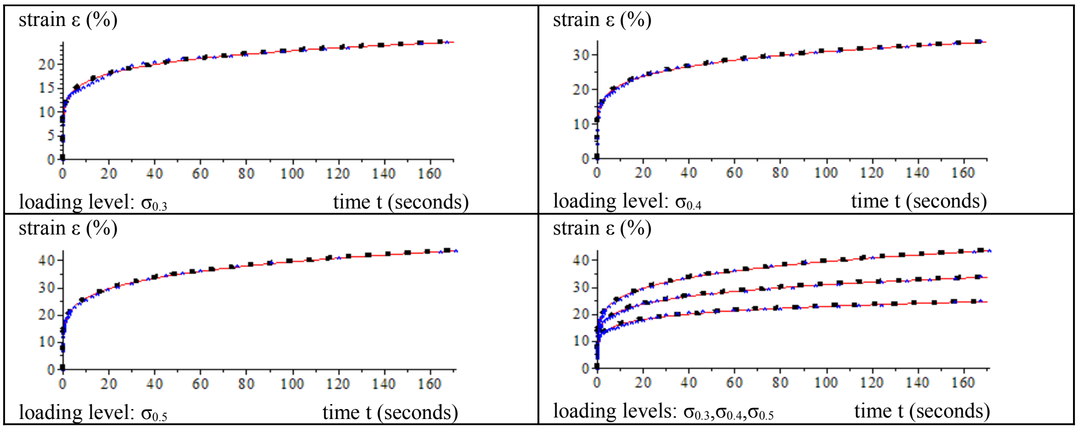

Figure 2. Results for pure polyamide (PA)

3.2. PA+UDD

The non-decision parameter values associated with polyamide (PA+UDD) are as follows. The parameter α is estimated as α = 0.83. The parameter E associated with $\varphi(\varepsilon) := E\varepsilon$ is determined as $E = 1008$. Loading levels are $\sigma_{0.3} = 15.90$, $\sigma_{0.4} = 21.20$, and $\sigma_{0.5} = 26.50$.

Table 2 gives the interpolating functions $I(t)$ associated with each data set, and also the optimal parameter estimates obtained as optimal solutions to (8).

	Interpolating Functions	Optimal Parameter Estimates	
Loading Level	$I(t) =$	β	λ
$\sigma_{0.3}$	$2.91939\ t^{0.2} + 16.79958\ t^{0.1} - 9.30827\ t^{0.05}$	0.02695	633.37560
$\sigma_{0.4}$	$26.28460\ t^{0.125} - 13.06354\ t^{0.0625}$	0.01340	607.21216
$\sigma_{0.5}$	$34.46006\ t^{0.125} - 18.58995\ t^{0.0625}$	-0.00403	580.75753

Table 2. Interpolating functions and optimal parameter estimates for polyamide (PA+UDD)

Fig.3 gives plots depicting wellness of fit of model $M_{\beta,\lambda}(t)$ with the experimental and interpolated data.

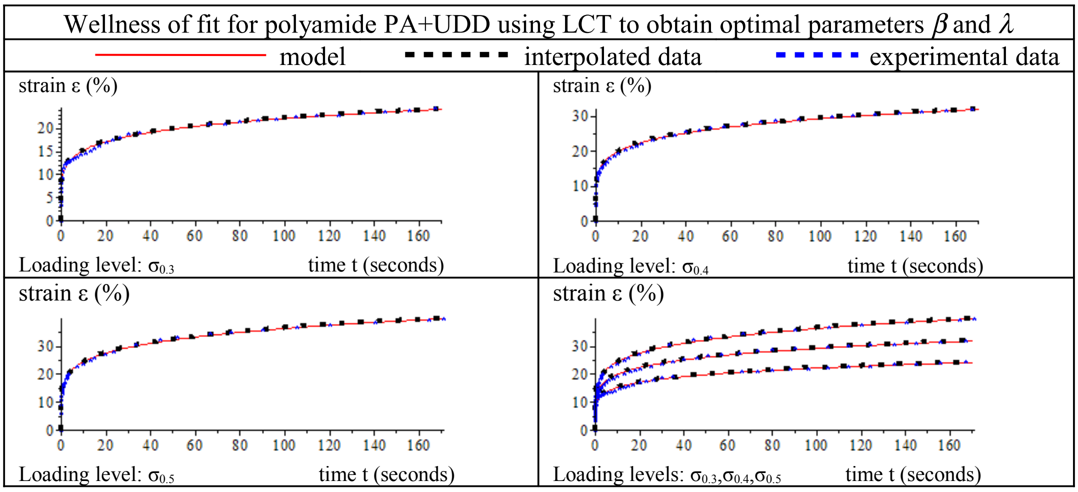

Figure 3. Results for polyamide (PA + UDD)

3.3. PA+CNT.

The non-decision parameter values associated with polyamide (PA+CNT) are as follows. The parameter α is estimated as $\alpha = 0.83$. The parameter E associated with the functional $\varphi(\varepsilon) := E\varepsilon$ is determined as $E = 1320$. The loading levels are defined as $\sigma_{0.3} = 18.72$, $\sigma_{0.4} = 24.96$, and $\sigma_{0.5} = 31.20$.

Table 3 gives the interpolating functions $I(t)$ associated with each data set, and also the optimal parameter estimates obtained as optimal solutions to (8). Fig. 4 gives plots depicting wellness of fit of model $M_{\beta,\lambda}(t)$ with the experimental and interpolated data.

	Interpolating Functions	Optimal Parameter Estimates	
Loading Level	$I(t) =$	β	λ
$\sigma_{0.3}$	$5.68600\ t^{0.2} + 3.11726\ t^{0.1}$	-0.00861	562.88010
$\sigma_{0.4}$	$113.44063\ t^{0.0667} - 102.36318\ t^{0.05}$	0.03109	605.66604
$\sigma_{0.5}$	$7.13975 - 7.13368\ e^{-0.05t} + 141.34010\ t^{0.0625} - 129.24869\ t^{0.05}$	0.00687	588.96000

Table 3. Interpolating functions and optimal parameter estimates for polyamide (PA+CNT)

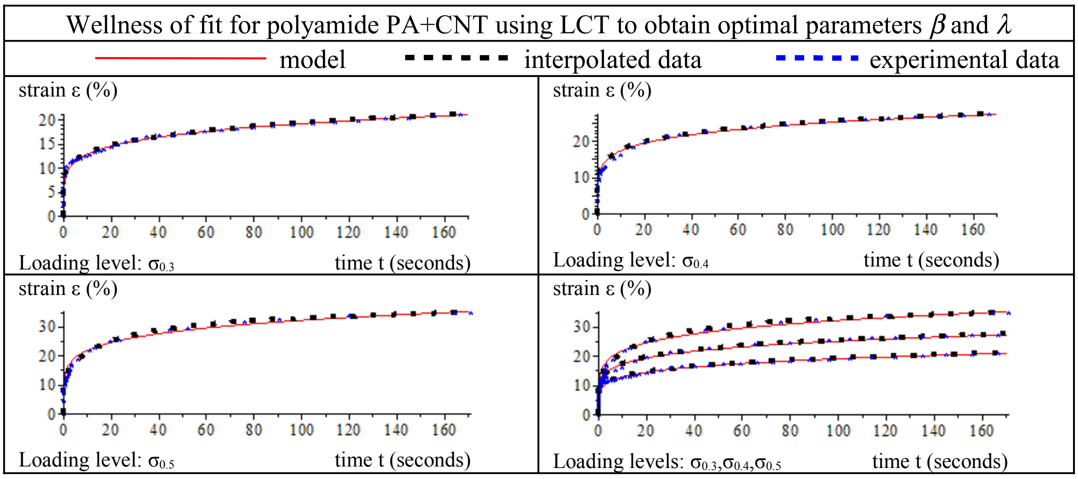

Figure 4. Results for polyamide (PA + CNT)

4. Concluding Remarks

As seen in the plots in Figs. 2-4, most of the parameters obtained for each material and each loading level yield creep models that fit the interpolating function well. The exception seems to be the material PA+CNT with loading level $\sigma_{0.5}$. It is unclear whether this is because of a poorly chosen sample region S_N for this material and loading level, or if the model $M_{\beta,\lambda}(t)$ is simply not able to fit the trend of the data well.

This work introduces the methodology of converting a difficult problem of finding optimal parameter estimates in the t domain into an alternative optimal parameter estimate problem in the Laplace transform s domain. The theoretical equivalence of the two problems is inferred from complex analysis theory presented in [10]. For the model and experimental cases considered, the Laplace transform optimization technique described in this work produces parameter estimates that fit the interpolated experimental data well.

Although the theoretical foundation is available for the use of Laplace transform optimization, there are practical computation questions that need further research. Numerical difficulty can arise from many sources when applying Laplace transform optimization. The first potential source of numerical difficulty arises from the computation of linear least squares. If the linear least squares problem is ill-conditioned, then slight change in the input data can result in great change in the optimal parameters and in the wellness of fit associated with optimal parameters. Details on this subject, and techniques for transforming the variable space to improve conditioning of the linear least squares problem are given in Section 4.4 of [11].

When equation (7) in the s domain is not perfectly satisfied for $s_i \in S_N$ for a given β and λ, the degree to which equation (5) in the t domain is not satisfied for the same β and λ is uncertain. The degree to which equation (5) is not satisfied seems to depend strongly on the choice of sampling region S_N used to set up problem (8). If the inverse LCT is thought of as a mapping taking in a function valued object in the s domain and outputting another function in the t domain, a notion of continuity of the inverse LCT (in terms of a function metric) is what allows for the possibility that (7) being “almost” satisfied means that (5) is “almost” satisfied. It is this notion of continuity that needs to be developed in future work.

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