NONLINEAR MODELING AND OPTIMIZATION OF PARAMETERS FOR VISCOELASTIC COMPOSITES AND NANOCOMPOSITES

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The hereditary mechanics accounting for the time dependent stress-strain relationship (also known as delay or memory effect) had started from Boltzman's work in the middle of 19th century and later was developed in fundamental research on integral equations by Volterra [1].The application of this mathematical theory to the modeling of deformation processes in the viscoelastic solids that are characterized by the memory of the history of loading had shown the tremendous potential for various engineering applications [2] involving ranging loading conditions like short/longterm creep, quasistatic loading, cyclic deformation for wide range of polymer based composites and as the recent studies show for the polymer based nanocomposites [3]. Consider the relationships between the following properties of viscoelastic solids:

- ε-denotes strain [%].
- σ-denotes load stress [MPa].
- t-denotes elapsed time [hours].

In particular, these solids have memory in the sense that load stress applied in the past manifests as present load stress.

The materials in question respond to stress in such a manner that stress applied in the past can affect 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 [5] to model the relationship between stress as a functional of strain

$$\varphi(\varepsilon(t)) = \sigma(t) + \int_0^t K(t-\tau)\sigma(\tau)d\tau \qquad (1)$$

where $\varphi(\varepsilon(t))$ is a response functional of ε (the so-called instantaneous loading diagram). In practice, this models the relations between time, stress and strain successfully for a wide range of materials such as polymers, metals, and composites [4]. This relationship appears visually in the graphs in Figure 1 for fixed time values t.

The most suitable kernel $K(t)$ is based on the exponential of arbitrary order function and for our purposes takes form

$$K(t) = \lambda \sum_{n=0}^{\infty} \frac{\beta^n t^{n(1-\alpha)}}{\Gamma[(1-\alpha)(n+1)]} \qquad (2)$$

The exponential of arbitrary order operators combine several important features

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

Initially, the goal of our work is to find the best way to estimate the kernel parameters $p = \{\lambda, \alpha, \beta\}$ that most accurately models the relation between stress, strain, and time with the use of (1).

With the above kernel, the integral in equation (1) can be evaluated, and so (1) becomes

$$\varphi(\varepsilon(t)) = \sigma(t)\left[1 + \lambda \sum_{n=0}^{\infty} \frac{(-\beta)^n t^{(1-\alpha)(n+1)}}{\Gamma[(1-\alpha)(n+1)+1]}\right] \qquad (3)$$

The parameter α is called the singularity parameter. Singularity reflects the rate of change for time $t \to 0$ of the stress-strain diagrams. All the parameter estimates correspond to the experimental test results for Nylon 6 [4]. The parameter α can be determined readily from the first term of the above infinite series (3) given as

$$\varphi(\varepsilon(t)) = \sigma(t)\left[1 + \frac{\lambda t^{(1-\alpha)}}{\Gamma[(1-\alpha)+1]}\right] \qquad (4)$$

and from information given in the isochronic creep curves of Figure 1. In such a manner, an estimate of $\alpha = 0.85$ is obtained.

Now consider finding the other two parameters λ and β for equation (3) that will model the relationship between stress, strain, and time as accurately as possible.

Start by restricting to the low loading level of $\sigma = 5MPa$. (This corresponds to curve #1 in Figure 2.) For this low loading level σ, and for strain $\varepsilon < 1\%$, the working assumption is that material response is linear, and therefore, one can obtain $\varphi(\varepsilon) = E\varepsilon$ and $\sigma_0 = E\varepsilon_0$. In turn, for this same loading level, ε as a function of t can be well-approximated by $\varepsilon(t) = at^b$ (Numerical results obtained: $a = 0.42, b = 0.079$.) Thus, substituting for $\varphi(\varepsilon) = E\varepsilon$, $\varepsilon = at^b$, and $\sigma = E\varepsilon_0$, equation (3) becomes

$$at^b = \varepsilon_0\left[1 + \lambda \sum_{n=0}^{\infty} \frac{(-\beta)^n t^{(1-\alpha)(n+1)}}{\Gamma[(1-\alpha)(n+1)+1]}\right]$$

Apply the Laplace-Carson transformation to both sides of the above equation to obtain

$$a\frac{\Gamma(1+b)}{s^b} = \varepsilon_0\left[1+\frac{\lambda}{s^{1-\alpha}+\beta}\right] \tag{5}$$

Thus, the question becomes one of determining parameters ε_0, λ, and β in the integral transform domain (α is known). Each choice of $\Delta s = \{s_1, s_2, s_3\}$ where s_1, s_2, s_3 are non-zero complex numbers determines a unique set of parameter values $p = \{\varepsilon_0, \lambda, \beta\}$. These are obtained by solving three equations of form (5) where s takes values s_1, s_2 and s_3 for each respective equation. When s_1, s_2, and s_3 are fixed, these three equations can be solved for closed-form expressions for $\varepsilon_0, \lambda, \beta$ with a, b, and α treated as known constants. Thus, the problem becomes one of finding the value $\Delta s = \{s_1, s_2, s_3\}$ defining the best parameter estimates.

Denote the most perfect model transformed from (3) by $\varepsilon[t_i, p^*]$ where the parameters p^* are the hypothetical best parameters. The search for the optimal parameters p can be formulated as the minimization of the following functional

$$F(p(\Delta s)) = \sum_{i=1}^{n}\left[\frac{\varepsilon[t_i, p(\Delta s)] - \varepsilon[t_i, p^*]}{\varepsilon[t_i, p^*]}\right]^2 \tag{6}$$

For example, for some value of Δs, we have $\lambda = 1.47$, $\beta = 0.13$, and $\varepsilon_0 = 0.2$ [4]. The wellness of fit for the model with obtained parameters is shown in Figure 2, where solid lines indicate the experimental results, and dashed lines the predicted results from the model. By construction, the model fits Diagram #1 well. However, there is clearly room for improvement in getting parameters that will allow a better fit for Diagrams #2 and #3 and to predict the mechanical behavior of different types of loading regimes.

The questions whose answers justify the use of standard optimization methods [6] can be summarized as follows:

(1) Where is the functional (6) defined?
(2) Where does the gradient of the functional (6) (with respect to Δs) exist?
(3) For what closed subsets of Δs is (6) a convex functional?

First, the behavior of the closed-form expressions for the parameters $p = \{\beta, \varepsilon_0, \lambda\}$ as functions of Δs are examined more closely. Preliminary results suggest that the parameter expressions and their subgradients w.r.t Δs are defined when s_1, s_2, s_3 are distinct. Furthermore, the parameters take real values when $0 < s_1 < s_2 < s_3$ are real or when one s value is positive real and the other two are complex conjugates of one another. Information obtained from the Hessian matrix of the closed-form expressions for the parameters and a selection of cross-sectional 3-D plots can give insight into the convexity of the functional and the general appearance of its optimal values. Once these questions are addressed, optimal parameter estimates are obtained for a given material and evaluated against wellness of fit with the experimental data and against other considerations for the soundness of the parameter estimates.

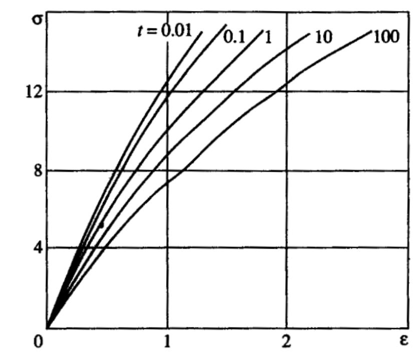

FIGURE 1. Isochonic creep diagrams

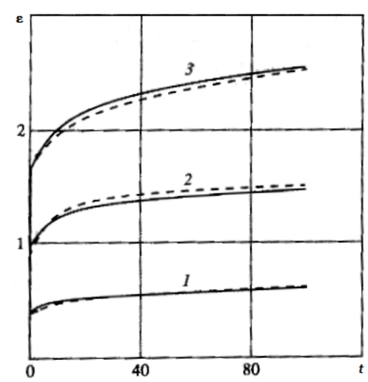

FIGURE 2. Progression of strain for three fixed levels of σ.

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