AN INVERSE PROBLEM IN VISCOELASTICITY

Lewis Thigpen, Gerald W. Hedstrom and Brian P. Bonner

Lawrence Livermore National Laboratory
Livermore, California 94550

ABSTRACT

Calculation of attenuation and dispersion spectra for a general anelastic body may be posed as an inversion problem. We observe the time-dependent strain due to "instantaneous" changes in stress in order to characterize the anelastic response. This experimental technique reaches a range of frequencies which is lower than that used in resonance bar experiments, but we can make only indirect measurement of the viscoelastic properties. We employ the most general anelastic model which states that the observed compliance is due to the summed effect of an arbitrary spectrum of mechanisms. The analysis requires the solution of Fredholm integral equations of the first kind. It is well known that this problem is ill-conditioned so that any numerical scheme will have to involve some smoothing to obtain accurate solutions. The present work employs Butler's method of constrained regularization which takes advantage of the fact that the solution is positive and uses data dependent smoothing. This work indicates that the imposition of the positivity constraint makes the computation of the solution much better conditioned. Computations with the method of constrained regularization employing near-optimal smoothing demonstrate its superiority over the method of Shapery for obtaining accurate solutions when the data are very noisy.

INTRODUCTION

The behavior of viscoelastic materials can be characterized in several different but related ways (Ferry, 1970; Christensen, 1971; Nowick and Berry, 1972). The most common measurements for the linear mechanical response are forced oscillation measurements as a function of frequency, and stress relaxation and creep measurements as a function of time. In this paper the mechanical response of a viscoelastic material is characterized by means of low strain creep and creep recovery experiments. The theory is based on the hypothesis that materials possess a complex structure and that viscoelasticity is reflected in the distribution function of the strain retardation time, τ, i.e., the retardation spectrum $X(\tau)$. The spectrum $X(\tau)$ is related directly to the creep function by a linear Fredholm integral equation of the first kind with an exponential kernel.

The principal objective of this paper is to present an example of the numerical inversion of the first kind integral equation for the distribution functions using a method of constrained regularization (Butler et al., 1981; Wahba, 1981). However, for completeness, we give some background information on the formulation of the integral equation for the distribution function in the next section.

DISTRIBUTION FUNCTION

Consider a state in which the stress is specified in terms of a unit step function

$$\sigma(t) = \sigma_o H(t) \quad , \tag{1}$$

where σ_o is the applied stress and $H(t)$ is the unit step function. The creep relation then becomes

$$\varepsilon(t) = J(t)\sigma_o \quad , \tag{2}$$

where $\varepsilon(t)$ is the strain and $J(t)$ is the creep function. The typical behavior in creep is initially a step change in time (instantaneous elasticity) followed by an increase over time with a decreasing slope (retarded elasticity or anelasticity) which may or may not approach an asymptote as t becomes large, depending on whether the material has undergone inelastic deformation or flow. Upon removal of the stress, there is an initial elastic recovery followed by anelastic recovery. The value of the creep function at large times after removal of the load determines the amount of inelastic deformation or flow that has taken place. For viscoelastic materials this permanent deformation gives a measure of the viscosity of the material.

The standard linear solid is the simplest mechanical model which mimics the behavior of the solid described above. It is a three parameter model consisting of a Voigt solid in series with a spring. Creep under constant stress then follows an exponential relation

$$J(t) = [J_o + \Delta J(1-e^{-t/\tau})]\ H(t) \quad , \tag{3}$$

where the time constant, τ, is the retardation time of strain and $\Delta J = J_\infty - J_o$. The model of a complex solid consists of a multiplicity of simple elements placed in series. The stress is the same in cell elements, whereas the total strain is the sum of the strains in each element. For this complex solid, the creep function is given by

$$J(t) = [J_o + \sum_{i=1}^{N} \Delta J_i\ (1-e^{-t/\tau_i})]H(t) \quad , \tag{4}$$

where N is the number of elements used to model the solid, $\Delta J = \Sigma\ \Delta J_i$ and τ_i is the time constant for each element. In the limit, the discontinuous system approaches a continuous one characterized by the distribution function, $X(\tau)$, of retardation times, τ. $X(\tau)d\tau$ is the contribution to the total creep which has a retardation time between τ and $\tau + d\tau$. This gives the creep function in terms of the distribution function

$$J(t) = J_o + \int_o^\infty X(\tau)\ (1-e^{t/\tau}\ )\ d\tau, \quad t \geq 0 \tag{5}$$

and

$$\int_o^\infty X(\tau)\ d\tau = \Delta J\ . \tag{6}$$

In solving for the spectrum $X(\tau)$, it is more convenient to rewrite Eq. (5) in the form

$$Kf = \int_o^\infty k(t,s)\ f(s)\ ds = g(t) \quad , \tag{7}$$

where we have used the following change of variables

$$s = 1/\tau\ , \tag{8}$$

$$X(\tau) = s^2 f(s), \tag{9}$$

and

$$g(t) = J(\infty) - J(t) . \tag{10}$$

Clearly, equation (7) is a Fredholm integral equation of the first kind with a Laplace kernel, i.e., $k(t,s) = e^{-st}$.

METHOD OF SOLUTION

An approximate solution of the integral equation

$$\int_0^\infty f(s)\, e^{-st}\, ds = g(t) \quad 0 < t < \infty , \tag{11}$$

where $g(t)$ has a bounded range $[g_0, g_N]$, may be obtained by one of two ways. One way is to write down an analytic expression for the distribution function $f(s)$ which allows calculation of the data function $g(t)$ and then comparing the calculated and measured curves. A second approach consists of deducing the distribution function from the experimentally given data set. However, a major difficulty is the sensitivity of the solution obtained to small perturbations in $g(t)$. Because of this property, the integral equation is referred to as ill-conditioned (Franklin, 1970; Tihonov, 1963). If $f(s)$ is replaced by

$$f(s) + A \sin \omega s,$$

then $g(t)$ is replaced by

$$g(t) + \frac{A\omega}{t^2 + \omega^2} .$$

For $\omega >> A$,

$$g(t) + \frac{A\omega}{t^2 + \omega^2} \simeq g(t).$$

This shows that large-amplitude, high frequency oscillations in the solution $f(s)$ correspond to imperceptible changes in the calculated data function $g(t)$.

To cope with the ill-conditioning, the integral equation is replaced by a stabilized problem

$$K_\alpha f_\alpha = g \tag{12}$$

which has the properties that $f_\alpha \to f_0$ as $\alpha \to 0$ and the sensitivity of f_α to small perturbations in g decrease as α increases. Here α is a positive constant. In this paper we use the Butler et al. (1981) method of constrained regularization to stabilize the problem. In that approach, the approximate solutions f_α are defined by

$$\text{Minimize } \psi(f) = \sum_1^N \left(\int f(s) \exp(-st_i)\, ds - g(t_i)\right)^2 + \alpha \|f\|^2 \quad ,$$

subject to the constraint $X(\tau) \geq 0$, i.e., $f(s) \geq 0$. Here $\|\cdot\|$ denotes the Euclidean R^N vector norm. The smoothing parameter α may be chosen according to the algorithm described in Butler et al. (1981). It should be noted that the Butler algorithm sometimes gives a value of α which is too large, and in that case α is chosen by experience. Alternatively, it is possible to choose α by Wahba's (1981) technique. Her technique is more reliable than Butler's, but it is also considerably more expensive. We have much more experience with Butler's method than with Wahba's. With the positivity constraint, the stabilized problem is equivalent to

$$f(s) = \max\left(0, \sum_1^N c_j e^{-st_j}\right), \tag{13}$$

$$Kf - g + \alpha c = 0 \ , \tag{14}$$

with

$$Kf = \int f(s)\, e^{-st}\, ds. \tag{15}$$

We now have a matrix equation

$$(M(f) + \alpha I)\, c = g \tag{16}$$

with

$$M_{ij}(f) = \int_{\text{supp } f} e^{-st_i}\, e^{-st_j}\, ds. \tag{17}$$

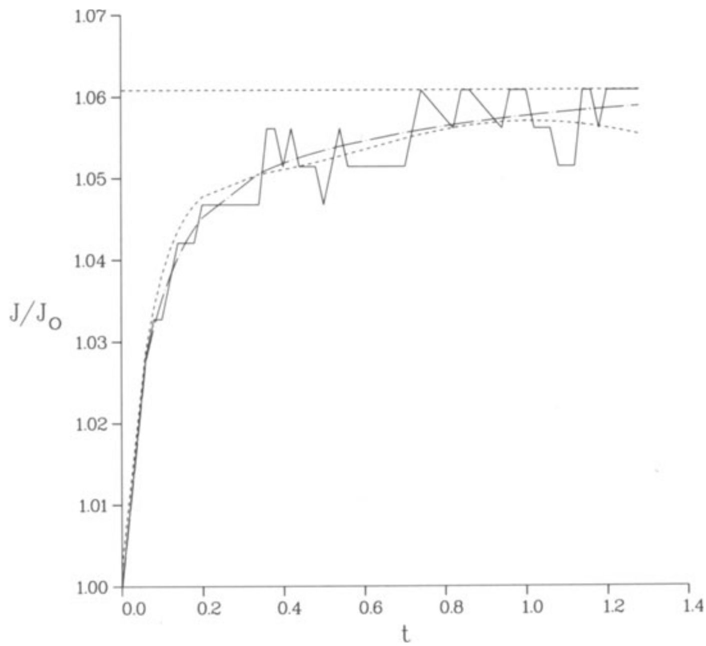

Figure 1. Normalized creep function.

Since M is symmetric and positive semi-definite, $(M+\alpha I)$ is non-singular. Note that c enters nonlinearly in the matrix equation so we solve it using Newton's method.

NUMERICAL EXAMPLE

Recent analysis has shown the method of constrained regularization gives good results to problems with known solutions (Thigpen et al. 1982). Here, we give an application of the method to invert spectra from the creep function for a commercial grade polymethylmethacrylate specimen. The experimental creep function for this material is depicted by a solid line in Fig. 1. The retardation spectrum obtained by the method of constrained regularization is illustrated by the solid line in Fig. 2. Here, we observe three peaks in the spectrum at approximately 0.0005 sec, 0.09 sec, and 0.6 sec, respectively, representing different retardation mechanisms. The two slower relaxations may be associated with the commonly observed β relaxation, an effect attributed to the rotation of $-COOCH_3$ side groups (McCrum et al., 1967). Anelastic effects associated with the presence of water appear in measurements at 20°C, but typically at periods much shorter than 0.0005 sec, the period of the broad peak in Fig. 2. Cautious interpretation is also advised since the sampling rate for the original data acquisition is 0.02 sec.

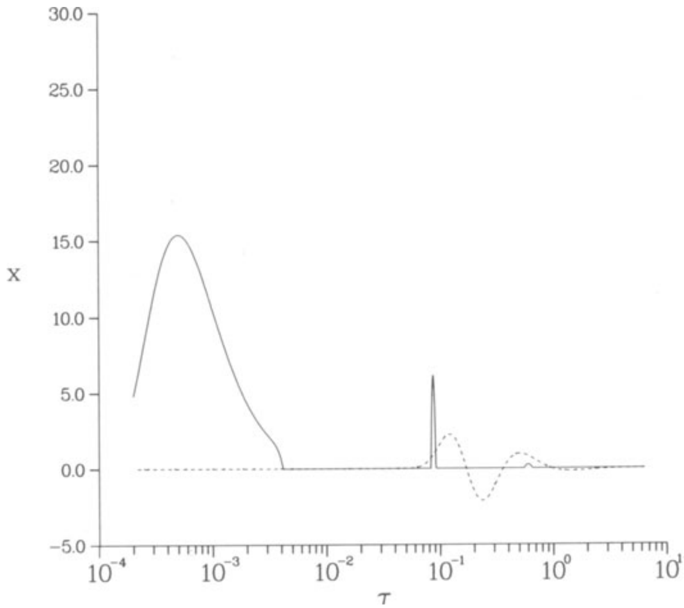

Figure 2. Distribution function.

The dashed curve depicted in Fig. 2 represents the spectrum obtained by approximating the data by a rational function, expanding it by partial fractions, and solving the integral equation by inspection. That is, we used essentially Shapery's (1962) method to solve Eq. (11). It is clear from the comparison of the two techniques that the ill-posed nature of the problem pollutes the solution obtained by Shapery's method. The peak in the spectrum at $\tau = 0.0005$ sec is not observed, and we know from physical grounds that the spectrum must be positive. Nevertheless, this method does give a solution which matches the data. See the dashed curve in Fig. 1. Here the comparison is as good as that obtained by constrained regularization (dot-dash curve, Fig. 1).

CONCLUSION

The method of constrained regularization does not guarantee an optimum solution to first kind integral equations. We have shown, however, that the technique provides significant improvements over more direct methods of solution such as the method of Shapery, particularly when the data are noisy. The main difficulty in implementing regularization is choosing a suitable smoothing parameter α. The method proposed by Butler et al. (1981) for choosing α gives reasonable results, but because the problem is so ill conditioned, this point deserves further investigation.

ACKNOWLEDGEMENT

This work was performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under Contract No. W-7405-ENG-48.

REFERENCES

Butler, J.P., Reeds, J.A. and Dawson, S.V., 1981, Estimating solutions of first kind integral equations with nonnegative constrains and optimal smoothing, SIAM J. Numer. Anal., 18, 381.

Christensen, R.M., 1971,"Theory of Viscoelasticity: An Introduction," Academic Press, New York.

Ferry, J.D., 1970, "Viscoelastic Properties of Polymers," John Wiley and Sons,.Inc., New York.

Franklin, J.N., 1970, Well posed stochastic extensions of ill-posed linear problems, J. Math. Anal. and Appl., 31, 682.

McCrum, N.G., Read, B.E. and Williams, G., 1967, "Anelastic and Dielectric Effects in Polymeric Solids," John Wiley and Sons, Inc., New York.

Nowick, A.S. and Berry, B.S., 1972, "Anelastic Relaxation in Crystalline Solids," Academic Press, New York.

Shapery, R.A., 1962, Approximate methods of transform inversion for viscoelastic stress analysis, Proc. 4th U.S. Nat. Cong. on Appl. Mech., 2, 1075.

Thigpen, L., Hedstrom, G.W. and Bonner, B.P., 1982, "Inversion of Creep Response for Retardation Spectra and Dynamic Viscoelastic Functions," Lawrence Livermore National Laboratory Report No. UCRL-87646, Livermore, CA.

Tihonov, A.N., 1963, Solution of incorrectly formulated problems and ahd regularization method, Soviet Meth. Dok., 4, 1035.

Wahba, G., 1981, "Constrained Regularization for Ill Posed Linear Operator Equations, with Applications in Meteorology and Medicine," University of Wisconsin, Department of Statistics, Technical Report No. 646, Madison, WI.

DISCUSSION

R.M. Bevensee (Lawrence Livermore National Laboratory): Did your solutions, in fact, have at least one eigenvector with zero eigenvalues?

L. Thigpen (Lawrence Livermore National Laboratory): Very close.

R.M. Bevensee: I suspect that if you took such an eigenvalue vector out and solved the problem, you'd get pretty nearly the right answer.

L. Thigpen: We thought of using the single value decomposition where you actually remove the single eigenvalues, but this is only one technique. There are numerous techniques for solving integral equations of the first kind, and we had chosen this method. We're going to try to pursue it as far as we can go, and then we may try other techniques.

D.O. Thompson (Ames Laboratory): Can you apply this to a heterogeneous system that has, say, many relaxation times?

L. Thigpen: In fact, we did make up some example problems. I have an example here where we have made up a problem with two distinct sets of relaxation times. This was an ideal problem again where I had a solution. We were able to resolve those peaks very clearly at the right relaxation time for the peak, and we then computed the attenuation because, again, we could solve for an exact solution. We computed the attenuation for noise levels of 2%, 10% and 20%. These were just arbitrary, because one of the questions is how much noise is going to be in the system. We got almost overlaying results for each case. The differences between the exact and the computer solutions were just characteristic of the noise, but they were very good solutions.