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The effect of kernel perturbations when solving the interconversion convolution equation of linear viscoelasticity

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ABSTRACT

In the study of linear viscoelastic materials, from measurements of the relaxation modulus $G(t)$, approximations to the corresponding creep compliance (retardation) modulus $J(t)$ are determined by solving the convolution interconversion equation

$$\int_0^t J(t-s)\,G(s)\,\mathrm{d}s = t, \quad t \geqslant 0.$$

By taking explicit account of the fact that $G(t)$ is a positive decreasing function, which automatically guarantees that $J(t)$ is positive increasing, new estimates are derived for the effect of perturbation in G on J. They allow an explicit assessment to be made of the well-posedness of the recovery of J from an approximation to G.

1. Introduction

The relaxation modulus $G(t)$ and creep compliance $J(t)$ of a linear viscoelastic material are often determined by conducting experiments on two separate instruments. However, as noted by various authors dating back to Gross [1] and Hopkins and Hamming [2], G and J satisfy, for $t \geq 0$, the interconversion relationship ([3], Chapters 3 and 4)

$$(J * G)(t) = \int_0^t J(t-s)G(s)\mathrm{d}s = (G * J)(t) = \int_0^t G(t-s)J(s)\mathrm{d}s = t. \tag{1}$$

Thus, an alternative approach is to determine either G or J from a single experiment and then obtain the other by solving the interconversion equation (1).

The interconversion equation is a Volterra convolution integral equation of the first kind. It is well known (cf. [4]) that such equations are improperly posed in the sense that, for some perturbation in the inhomogeneous term, arbitrary large perturbations pollute the solution (J if the relaxation modulus G has been measured, or G if the creep modulus J is given). However, because the right hand side t of Eq. (1) is exact, the more interesting and relevant question is that of the improperly posed nature of (1) with respect to perturbation in either the kernel J or G.

It is also known that numerical schemes, that have been constructed for the approximate solution of the interconversion equation, can exhibit ill-conditioning. This has generally been attributed to the improperly posed nature of (1). As a consequence, some authors have proposed numerical schemes based on second-kind Volterra integral equations obtained by differentiating (1) (see for example [5]). Nikonov [6] propose a new experiment from which the relaxation modulus and creep compliance could be computed via the numerical solution of second-kind Volterra integral equations. However, it

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is incorrect to conclude that a first-kind Volterra equation, such as (1), is poorly conditioned if, on the basis of numerical experimentation, numerical methods for its solution behave in an unstable manner.

In fact, we show in this work that, with respect to perturbations in G, the determination of J using the interconversion equation (1) is well-posed. This is achieved by analysing the situation where the creep compliance J is to be calculated from an estimate of the relaxation modulus G. There are two key reasons for restricting attention to the G-to-J interconversion. Firstly, in a series of papers [7–9], it has been established theoretically that the interconversion from G to J is guaranteed to be stable, while the interconversion from J to G can be unstable. Secondly, as a minimum, it must be assumed that G is positive and decreasing [10]; namely,

$$G \in C^1[0,\infty), \quad G(t) > 0, \qquad G'(t) = \frac{dG}{dt} < 0, \quad 0 \leqslant t < \infty.$$

As shown explicitly below, such a choice for G guarantees that the corresponding J is positive and increasing [11], which is consistent with the minimal conditions that J must satisfy. However, the converse does not hold, because a positive and increasing J does not guarantee that G is positive and decreasing. Consequently, some appropriate conditions must be imposed on the growth of J in order to ensure that G is decreasing. This is discussed in some detail in [11,12].

Since, in rheology applications, G (or J) will only be known approximately, it is important to know how perturbations in G (or J) affect the recovery of J (or G) by solving the interconversion equation (1). An analysis [7–9] of the effect of perturbations when solving the interconversion equation established theoretically the stability of the recovery of J from G and the potential instability of G from J. It was subsequently shown [11] how this analysis could be generalized to analysing the effect of perturbations in the kernel on the solution of first-kind convolution Volterra equations. The results given in the sequel are a consequence of this generalization applied to the interconversion equation (1).

Let $\tilde{G}$ denote the estimate (approximation), determined from some appropriate experiment, of G. Following standard rheological practice, $\tilde{G}$ will have been chosen to have a similar structure to G; namely, as a minimum,

$$\tilde{G} \in C^1[0,\infty), \quad \tilde{G}(t) > 0, \qquad \tilde{G}'(t) = \frac{d\tilde{G}}{dt} < 0. \tag{2}$$

Consequently, $\delta G = \tilde{G} - G$ represents the perturbation (or error) in G, with the corresponding approximate creep compliance $\tilde{J} = J + \delta J$ satisfying the interconversion relationship (1)

$$(\tilde{G} * \tilde{J})(t) = (G + \delta G) * (J + \delta J)(t) = t, \tag{3}$$

from which it follows that

$$G * \delta J = -\tilde{J} * \delta G,$$

and, hence, on convolving this last equation with J, invoking (1) and differentiating the resulting equation twice, one obtains

$$\delta J = -\frac{d^2}{dt^2}(J * \tilde{J} * \delta G)(t). \tag{4}$$

It is this equation that is utilized below to derive absolute and relative error estimates for δJ in terms of δG.

The work has been organized in the following manner. A series of lemmas are proved in Section 2 which are then used to prove the stability results of Section 3. An interpretation of the results from a linear viscoelastic perspective is given in Section 4.

2. Preliminaries

The lemmas below are derived for general functions a, b, c, and d. They are then applied to Eq. (4) in the next section in order to derive the stability results. As above, the prime superscript is used to denote differentiation with respect to t; namely, $a' = da/dt$ and $a'' = d^2a/dt^2$.

Lemma 1. *Let $a, b, c \in C^1[0,\infty)$; then*

$$|(a * (bc))(t)| \leqslant (|a| * |b|)(t) \max_{0\leqslant s\leqslant t} |c(s)|,$$

where $C^1[0,\infty)$ denotes the set of functions defined on the interval $[0,\infty)$ which have continuous first derivatives.

Lemma 2. *Let $a, b \in C^1[0,\infty)$, $a, b \geqslant 0$, $a', b' \geqslant 0$ and $c \in C[0,\infty)$. Then*

$$(a * |c|)' \geqslant 0,$$
$$(a * b)' \leqslant a(t)b(t),$$
$$(a * b)'' \geqslant 0,$$
$$(a * b * |c|)'' \geqslant 0.$$

Proof. Under the given regularity, the proofs reduce to sequentially performing the algebraic steps listed below.

$$(a * |c|)' = a(0)|c(t)| + (a' * |c|)(t) \geqslant 0,$$
$$(a * b)' = a(0)b(t) + (a' * b)(t) \leqslant a(0)b(t) + b(t)(a' * 1)(t) = a(t)b(t),$$
$$(a * b)'' = a(0)b'(t) + b(0)a'(t) + (a' * b')(t) \geqslant 0,$$
$$(a * b * |c|)'' = a(0)b(0)|c(t)| + a(0)(b' * |c|)(t) + b(0)(a' * |c|)(t) + (a' * b' * |c|)(t) \geq 0. \quad \square$$

Lemma 3. *Let $a, b \in C^1[0, \infty)$, $a, b \geqslant 0$, $a', b' \geqslant 0$ and $c, d \in C[0, \infty)$. Then*

$$|(a * b * (cd))''| \leqslant (a * b * |c|)'' \max_{0 \leqslant s \leqslant t} |d(s)|.$$

Proof. Under the given regularity, the proofs reduce to sequentially performing the algebraic steps listed below.

$$\begin{aligned} |(a * b * (cd))''| &= |a(0)b(0)c(t)d(t) + a(0)(b' * (cd))(t) + b(0)(a' * cd)(t) + (a' * b' * (cd))(t)| \\ &\leqslant \{a(0)b(0)|c(t)| + a(0)(b' * |c|)(t) + b(0)(a' * |c|)(t) + (a' * b' * |c|)(t)\} \max_{0 \leqslant s \leqslant t} |d(s)| \\ &= (a * b * |c|)'' \max_{0 \leqslant s \leqslant t} |d(s)|, \end{aligned}$$

where the last inequality is established by applying Lemmas 1 and 2. $\square$

Lemma 4. *Let $a, b \in C^1[0, \infty)$, $a, b \geqslant 0$, $a', b' \geqslant 0$ and $c \in C[0, \infty)$. Then*

$$\int_0^t \left| \frac{\mathrm{d}^3}{\mathrm{d}s^3}(a * b * c)(s) \right| \mathrm{d}s \leqslant (a(t)b(t) - a(0)b(0))|c(0)| + a(t)b(t) \int_0^t |c'(s)|\mathrm{d}s.$$

Proof. The first step involves determining the following upper bound:

$$\begin{aligned} \left| \frac{\mathrm{d}^3}{\mathrm{d}t^3}(a * b * c)(t) \right| &= |c(0)(a * b)'' + (a * b * c')''| \\ &\leqslant |c(0)|(a * b'') + (a * b * |c'|)''. \end{aligned}$$

Integration of this last relationship then yields

$$\begin{aligned} \int_0^t \left| \frac{\mathrm{d}^3}{\mathrm{d}s^3}(a * b * c)(s) \right| \mathrm{d}s &\leqslant \int_0^t [|c(0)|(a * b)''(s) + (a * b * |c'|)''(s)]\mathrm{d}s \\ &= |c(0)|[(a * b)'(t) - a(0)b(0)] + (a * b * |c'|)'(t) \\ &\leqslant [a(t)b(t) - a(0)b(0)]|c(0)| + a(t)b(t) \int_0^t |c'(s)|\mathrm{d}s. \quad \square \end{aligned}$$

Lemma 5. *Let $a \in C^2[0, \infty)$, $a > 0$ and $a' < 0$. Then*

$$(a * b)(t) = t \tag{5}$$

has a solution $b \in C^1[0, \infty)$. Furthermore, $b > 0$, $b' > 0$ and $ab \leqslant 1$.

Proof. Differentiating (5) yields

$$a(0)b(t) + (a' * b)(t) = 1 \tag{6}$$

which is a second-kind Volterra integral equation. Standard theory for second-kind Volterra integral equations ensures the existence of a solution $b \in C[0, \infty)$. Furthermore,

$$b(0) = 1/a(0) > 0.$$

Suppose that $b(t) > 0$ for $0 < t \leqslant t^*$ and $b(t^*) = 0$. Then,

$$a(0)b(t^*) = 1 - (a' * b)(t^*) \geqslant 1 > 0,$$

which contradicts the assumption that $b(t^*) = 0$. Thus, $b(t) > 0$ for all t. Differentiating (6) yields

$$a(0)b'(t) + (a' * b')(t) = -b(0)a'(t),$$

and an argument similar to that given above ensures the existence of a solution $b' \in C[0, \infty)$ with $b' > 0$. From (6),

$$1 = a(0)b(t) + (a' * b)(t) \geqslant a(0)b(t) + (a' * 1)(t)b(t) = a(t)b(t). \quad \square$$

3. Stability results

Through appropriate choices for a, b, c and d in Lemma 3, and the subsequent utilization of the other lemmas and equations, various stability results can be derived. Because of the complete monotonicity of G, $\tilde{G}$, J' and $\tilde{J}'$, the conditions given in the above lemmas will be automatically satisfied.

Initially, in the first theorem, absolute and relative error bounds for δJ are given in terms of the absolute and relative values of δG, respectively.

Theorem 1.

$$|\delta J(t)| \leqslant J(t)\tilde{J}(t) \max_{0\leqslant s\leqslant t} |\delta G(s)|, \tag{7}$$

$$\left|\frac{\delta J(t)}{J(t)}\right| \leqslant \max_{0\leqslant s\leqslant t} \left|\frac{\delta G(s)}{\tilde{G}(s)}\right|, \tag{8}$$

$$\left|\frac{\delta J(t)}{\tilde{J}(t)}\right| \leqslant \max_{0\leqslant s\leqslant t} \left|\frac{\delta G(s)}{G(s)}\right|. \tag{9}$$

Proof. The first result follows on applying Lemma 3 to the right hand side of (4) with $a = J$, $b = \tilde{J}$, $c = 1$, $d = \delta G$ and then applying the second inequality in Lemma 2. The second result follows on first applying Lemma 3 to the right hand side of (4) with $a = J$, $b = \tilde{J}$, $c = \tilde{G}$, $d = \delta G/\tilde{G}$ and then using the fact that $(J * \tilde{J} * \tilde{G})'' = J$. The third result follows on first applying Lemma 3 to the right hand side of (4) with $a = J$, $b = \tilde{J}$, $c = G$, $d = \delta G/G$ and then using the fact that $(J * \tilde{J} * G)'' = \tilde{J}$. □

The well-posedness of the recovery of J from G using (1) is an automatic consequence of this theorem. Since $J\tilde{J}$ is bounded, even though it can be quite large, the absolute error $|\delta J|$ is bounded, because $|\delta G(s)|$ is bounded. The relative error results are much stronger. The two relative error estimates for J are bounded by the size of the corresponding relative error estimates for G. Because of the decreasing nature of $G(t)$, the relative error estimates for G of Eqs. (8) and (9) will be bounded if δG and $\tilde{G}$ decay in a similar manner to G.

In a rheological application, once estimates $\tilde{G}$ and $\tilde{J}$ have been obtained for G and J from available stress–strain measurements, the corresponding Boltzmann causal integral equations of linear viscoelasticity

$$\sigma(t) = \gamma(0)\tilde{G}(t) + \int_0^t \tilde{G}(t-s)\dot{\gamma}(s)\mathrm{d}s, \qquad \dot{\gamma}(t) = \frac{\mathrm{d}\gamma(t)}{\mathrm{d}t}, \tag{10}$$

and

$$\gamma(t) = \sigma(0)\tilde{J}(t) + \int_0^t \tilde{J}(t-s)\dot{\sigma}(s)\mathrm{d}s, \qquad \dot{\sigma}(t) = \frac{\mathrm{d}\sigma(t)}{\mathrm{d}t}, \tag{11}$$

must be evaluated in order to predict the stresses $\sigma(t)$ and strains $\gamma(t)$ for various scenarios of practical interest. Representative error estimates for the evaluation of such stresses and strains can be derived through the use of appropriate integrated error estimates.

In fact, Lemma 4 can be used to derive such an error estimate for the rate of change of δJ.

Theorem 2.

$$\int_0^t \left|\frac{\mathrm{d}}{\mathrm{d}s}\delta J(s)\right| \mathrm{d}s \leqslant (J(t)\tilde{J}(t) - J(0)\tilde{J}(0))|\delta G(0)| + J(t)\tilde{J}(t)\int_0^t |(\delta G)'(s)|\mathrm{d}s.$$

Proof. The result follows on applying Lemma 4 to the right hand side of (4) with $a = J$, $b = \tilde{J}$ and $c = \delta G$. □

The importance of this result is that it makes explicit the rate of change of δJ in terms of the rate of change in δG. It lends support to the need to choose an approximation $\tilde{G}$ for G which ensures that $(\delta G)'$ is well-behaved.

4. Interpretation and conclusions

In applied and industrial rheological applications, the need arises to predict the stress–strain response of complex flow and deformation scenarios. The first step is the recovery of estimates for G and J from laboratory instrument measurements. Here, Theorem 1 has been derived to establish that the recovery of J from G is well-posed. This complements the earlier results of [7–9] concerning the stability of the recovery of J from G. Together, these two results imply that, from a technical perspective, only instrumental measurements of stress as a function of strain are required to recover an estimate of G with the corresponding estimate of J being derived computationally by solving the interconversion relationship (1).

For a given flow and deformation application, once estimates for G and J have been derived, the predictions of the stress–strain responses for more complex scenarios are derived by evaluating the corresponding Boltzmann equations (10) and (11) of linear viscoelasticity. The integrated error estimate of the type derived in Theorem 2 can be utilized to derive error estimates for the evaluation of the Boltzmann equations.

The results indicate that the behaviour of δJ is strongly controlled through the choice of $\tilde{G}$ as this determines the form of $\delta G = \tilde{G} - G$. In addition, it is clear that the choice of $\tilde{G}$ should be such as to ensure that it and G behave in a similar manner asymptotically for increasing t.

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