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An Improved Numerical Interconversion for Creep Compliance and Relaxation Modulus

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Synopsis

An improved method for the numerical evaluation of the convolution integral in the relationship between creep compliance and relaxation modulus is discussed. The better approximation is obtained by the assumption that both functions can be assumed to be linear within a series of increasing time intervals which do not change as the calculation progresses. The calculation is carried out on both hypothetical and real examples which substantiates its applicability and accuracy.

INTRODUCTION

It is well known that as a direct consequence of the superposition principle, the stress and strain in a linear viscoelastic material may be related to each other through the relaxation modulus or creep compliance:[1,2]

$$L[\sigma(t)] = sL[G(t)]L[\epsilon(t)] \tag{1}$$

$$L[\epsilon(t)] = sL[J(t)]L[\sigma(t)] \tag{2}$$

or

$$L[G(t)]L[J(t)] = 1/s^2 \tag{3}$$

where L indicates the Laplace transform (see, for example, Churchill[3]):

$$L[X(t)] = \int_0^\infty X(t)e^{-st}dt. \tag{4}$$

Alternately, eq. (3) may be expressed in the form of a convolution integral

$$\int_0^t J(t - \tau)G(\tau)d\tau = t \tag{5}$$

or equivalently

$$\int_0^t G(t - \tau)J(\tau)d\tau = t. \tag{6}$$

Another form of this relationship may be derived by using the fact that

$$L[F'(t)] = sL[F(t)] - F(0) \tag{7}$$

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where $F(t)$ is an appropriate well-behaved function, $F'(t)$ is its derivative, and $F(0)$ is its value at $t = 0$. When this is substituted into eq. (3), and replacing $F(t)$ with $G(t)$ or $J(t)$, we obtain

$$L[G'(t)]L[J(t)] = 1/s - G(0)L[J(t)] \tag{8}$$

or equivalently

$$L[J'(t)]L[G(t)] = 1/s - J(0)L[G(t)] \tag{9}$$

which also can be expressed in a convolution integral form

$$\int_0^t J'(t - \tau)G(\tau)d\tau = 1 - J(0)G(t) \tag{10}$$

or

$$\int_0^t G'(t - \tau)J(\tau)d\tau = 1 - G(0)J(t). \tag{11}$$

Two more equivalent representations can be obtained by switching the roles of the functions inside each of the integrals. In any situation where one wishes to convert from one viscoelastic function to the other or where one has time-dependent stress and strain,[4] these types of integral equations must ultimately be evaluated.

A numerical solution to eqs. (5) and (6) has been performed in the past.[5,6] This method works very well considering the approximations made. It does suffer from drawbacks. The calculated values are not those of any particular time, but are a mean value within an interval of time, and the conversion of compliance to modulus is extraordinarily sensitive to "noise" in the data. The following sections contain a more sophisticated numerical evaluation of the integral equations involved. It is free of the drawbacks of the previous treatment and has proven itself to be practical for almost any type of data.

NUMERICAL SOLUTION

It has been found through experience and mathematical reasoning that of the many equations presented in the previous section, different forms are to be used depending on which is the known function. If modulus, $G(t)$, is known and compliance, $J(t)$, is to be calculated, eq. (6) should be employed. If compliance is known, eq. (10) is the most suitable. The known function always occupies the inverse coordinate position, $G(t - \tau)$ or $J(t - \tau)$, in order to avoid restrictions on the times at which the known function is tabulated. The evaluation of the integral on the left of both eqs. (6) and (10) is essentially the same for both forms and will be presented in the general form

$$\int_0^t X(t - \tau)Y(\tau)d\tau \tag{12}$$

where X is the known function and Y is that to be calculated.

Actually, X is not known at all times, but is tabulated at discrete times. We introduce the notation $X[t(i)]$ as the value of X at $t(i)$ for $i = 1$ to n, where $t(1) = 0.0$, and *assume* that X can be accurately represented by a linear relationship between $t(i)$ and $t(i - 1)$.

This method can handle time intervals chosen in any way, but has been formulated for the specific case when $t(i + 1) - t(i) > t(i) - t(i - 1)$. This is necessary in order to cover the many decades of logarithmic time which compliance or modulus data normally cover. In the case when $t(i + 1) - t(i) = t(i) - t(i - 1)$, the entire calculation is simplified greatly. Details of this can be supplied on request. If modulus is the known function, then $X[t(i)] = G[t(i)]$ at each time. If compliance is known, the J values must be calculated using

$$X[t(i)] = J'[t(i)] = \frac{J[t(i + 1)] - J[t(i - 1)]}{t(i + 1) - t(i - 1)} \tag{13}$$

for $i = 2$ to $n - 1$, and

$$X[t(1)] = J'[t(1)] = \frac{J[t(2)] - J[t(1)]}{t(2) - t(1)} \tag{14}$$

$$X[t(n)] = J'[t(n)] = \frac{J[t(n)] - J[t(n - 1)]}{t(n) - t(n - 1)}. \tag{15}$$

We then must perform the integration of integral (12) between $t = 0$ and $t = t(k)$ for $k = 2$ to n.

Thus, integral (12) becomes

$$\int_0^{t(k)} X[t(k) - \tau]Y(\tau)d\tau. \tag{16}$$

The linear relationships which we will use to approximate the functions within the specific time intervals are

$$Y(\tau) = Y[t(i - 1)] + \frac{\tau - t(i - 1)}{t(i) - t(i - 1)} \{Y[t(i)] - Y[t(i - 1)]\} \tag{17}$$

where $t(i - 1) \leq \tau \leq t(i)$, and

$$X(t(k) - \tau) = X(t(q)) + \frac{\tau - t(k) + t(q)}{t(q) - t(q - 1)} \{X(t(q - 1)) + X(t(q))\} \tag{18}$$

where $t(k) - t(q) \leq \tau \leq t(k) - t(q - 1)$. The correctness of these expressions can be verified using Figure 1, which shows hypothetical $Y(\tau)$ and $X(t(k) - \tau)$ functions with $k = 4$. We now define $tw(j)$, where $j = 1$ to $2k - 2$, as a time vector which contains all the times $t(i)$, $i = 1$ to k, and $t(k) - t(i)$, $i = 2$ to $k - 1$, in order of their magnitude (see Fig. 1). The purpose of choosing time intervals in this way is to maintain a reasonably constant degree of approximation of the actual functions by the

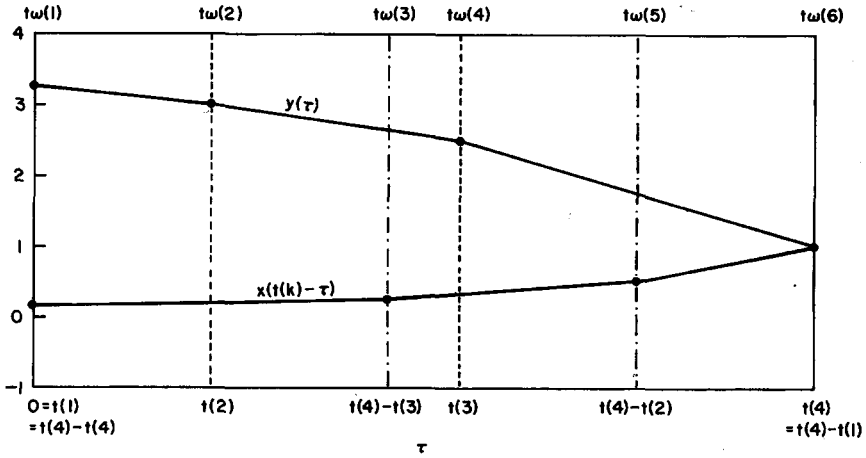

Fig. 1. Example showing how time intervals are marked off using a hypothetical Y and X with $k = 4$.

following summation of integrations, which is a direct consequence of integral (16):

$$\sum_{j=2}^{2k-2} \int_{tw(j-1)}^{tw(j)} X(t(k) - \tau)Y(\tau)d\tau. \tag{19}$$

The substitution of these linear functions of X and Y in quantity (19) thus replaces the product of the integral of the linear X function over each time interval and a mean value of Y for that interval as specified in the algorithm of reference 5. We also make the specification that $tw(kq)$ is the time at which the last value of Y is known. For example, in Figure 1 we would be calculating the value of $Y(t(4))$, and the last-known value of Y would be at $t(3)$ which is $tw(4)$, and therefore $kq = 4$. The summation of eq. (19) is therefore broken into two parts:

$$\sum_{j=2}^{kq} \int_{tw(j-1)}^{tw(j)} X(t(k) - \tau)Y(\tau)d\tau + \sum_{j=kq+1}^{2k-2} \int_{tw(j-1)}^{tw(j)} X(t(k) - \tau)Y(\tau)d\tau. \tag{20}$$

The first is the sum of all the integrals for which we know all values of both functions. The second part contains the integrals in which $Y(t(k))$ is the only unknown. Of course, the previous Y values have already been calculated starting at $k = 2$.

Before proceeding further, the following simplifying substitutions can be used in eqs. (17) and (18):

$$Z1 = \frac{X(t(q-1)) - X(t(q))}{t(q) - t(q-1)} \tag{21}$$

$$Z2 = \frac{Y(t(i)) - Y(t(i-1))}{t(i) - t(i-1)} \tag{22}$$

$$Z3 = Y(t(i-1)) - t(i-1)\cdot Z2 \tag{23}$$

$$Z4 = X(t(q)) + (t(q) - t(k))\cdot Z1. \tag{24}$$

When eqs. (17) and (18) are substituted into the integrals of the first summation of quantity (20), the following result is obtained upon integration:

$$\sum_{=2}^{kq} [Z3\cdot Z4\cdot(tw(j) - tw(j-1)) + (Z4\cdot Z2 + Z3\cdot Z1)\cdot(tw(j)^2 - tw(j-1)^2)/2 + Z2\cdot Z1\cdot(tw(j)^3 - tw(j-1)^3)/3] \tag{25}$$

which we will designate ZZ. The second summation yields the following:

$$Y(t(k-1))\cdot \sum_{j=kq+1}^{2k-2} [Z4\cdot(tw(j) - tw(j-1)) + Z1\cdot(tw(j)^2 - tw(j-1)^2)/2] + Z2\cdot \sum_{j=kq+1}^{2k-2} [Z4\cdot(tw(j)^2 - tw(j-1)^2)/2 + Z1\cdot(tw(j)^3 - tw(j-1)^3)/3 + t(k-1)\cdot(Z4\cdot(tw(j) - tw(j-1)) + Z1\cdot(tw(j)^2 - tw(j-1)^2)/2)] \tag{26}$$

which we will designate

$$Y(t(k-1))\cdot ZV + Z2\cdot ZW. \tag{27}$$

Quantity 20 thus becomes

$$ZZ + Y(t(k-1))\cdot ZV + \frac{Y(t(k)) - Y(t(k-1))}{t(k) - t(k-1)}\cdot ZW. \tag{28}$$

At this point the derivation differs according to the identity of X as discussed previously. If X is G, then quantity (28) is set equal to $t(k)$ and solving for $Y[t(k)]$, we obtain

$$Y[t(k)] = \frac{t(k) - ZZ - Y(t(k-1))\cdot ZV + \dfrac{Y(t(k-1))}{(t(k) - t(k-1))}\cdot ZW}{ZW/(t(k) - t(k-1))}. \tag{29}$$

If X is J', the quantity (28) is set equal to $1 - X(1)Y(t(k))$, and

$$Y(t(k)) = \frac{1 - ZZ - Y(t(k-1))\cdot ZV + \dfrac{Y(t(k-1))}{(t(k) - t(k-1))}\cdot ZW}{X(t(1)) + ZW/(t(k) - t(k-1))} \tag{30}$$

Given the first value of Y,

$$Y(t(1)) = 1/X(t(1)), \tag{31}$$

each succeeding value can then be calculated.

EXAMPLES

Figure 2 shows the three curves obtained from the hypothetical relaxation equation

$$G(t) = e^{-t^B} \tag{32}$$

for the values of B indicated on the figure; 10 and 20 points per decade of logarithmic time were used for $B = 0.2$ and 0.5, respectively. For $B = 1.0$, the number per decade varied from 10 at log time $= -3$ to 200 at log time $= 2$. This was necessary because of the severe decay of this function. As in the derivation, the functions were assumed to be linear within each time interval. Figure 3 shows the corresponding $J(t)$ curves as calculated using eq. (29). In the case $B = 1.0$, $J(t)$ can be expressed analytically as

$$J(t) = 1 + t. \tag{33}$$

The conversion from $G(t)$ to $J(t)$ was accurate to within 0.02% at log $t = 1.0$. $G(t)$ was then recalculated from the $J(t)$ data using eq. (30). Figure 4 shows the absolute per cent error in the data which were returned from the calculated $J(t)$ curves using eq. (30) as a function of the magnitude of the original $G(t)$. The difference between the $B = 0.5$ and $B = 0.2$ conversions is due to the number of points taken per decade of logarithmic time, and the $B = 0.2$ could be improved significantly by using more points.

Figures 5, 6, and 7 show the relaxation moduli and the calculated creep compliance curves for three experimentally determined master curves.

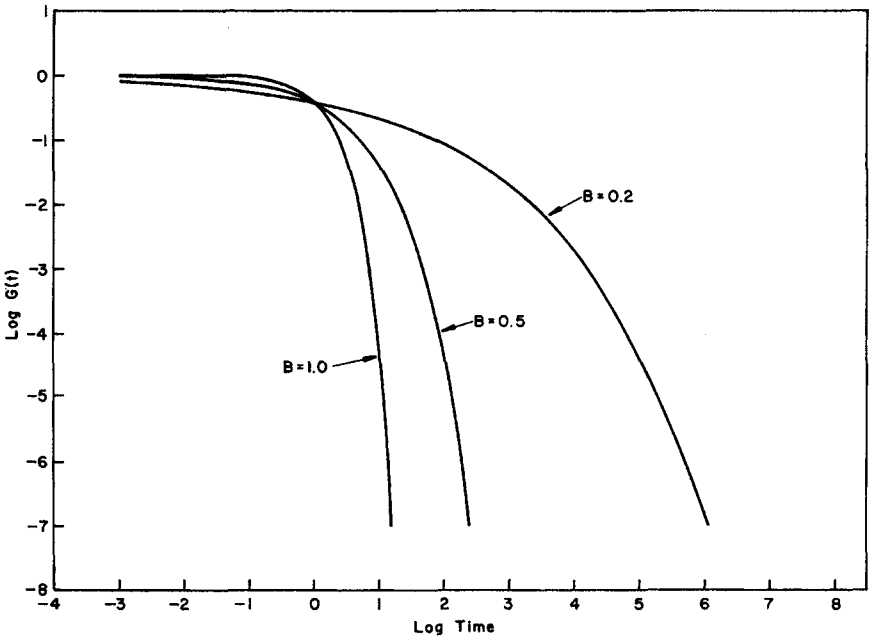

Fig. 2. Logarithm of $G(t)$ vs. log time for three analytical relaxation functions.

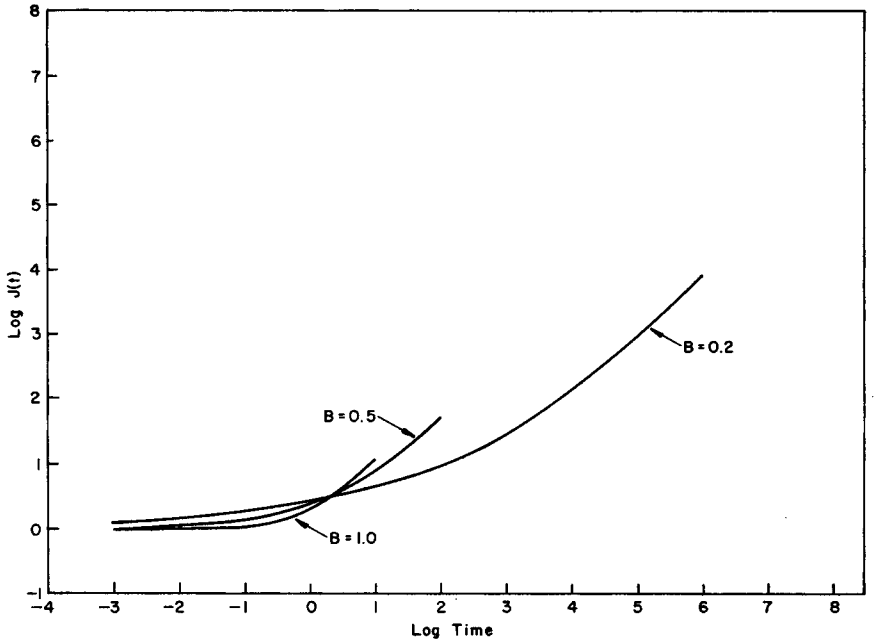

Fig. 3. Creep functions corresponding to relaxation functions of Fig. 2 as calculated by eq. (29).

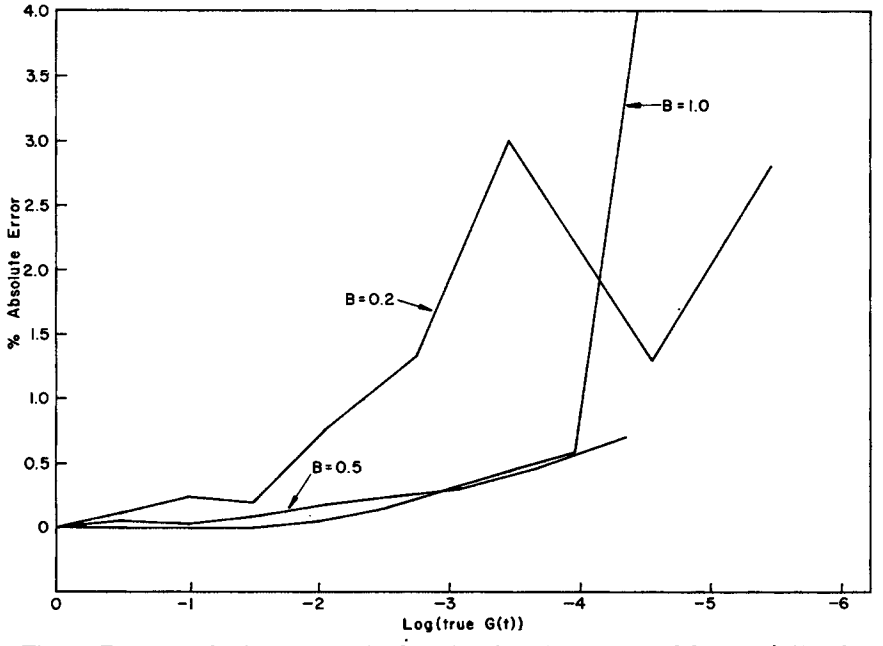

Fig. 4. Per cent absolute error of relaxation functions returned by eq. (30) using data from eq. (29) with respect to original data plotted as a function of negative logarithm of the original.

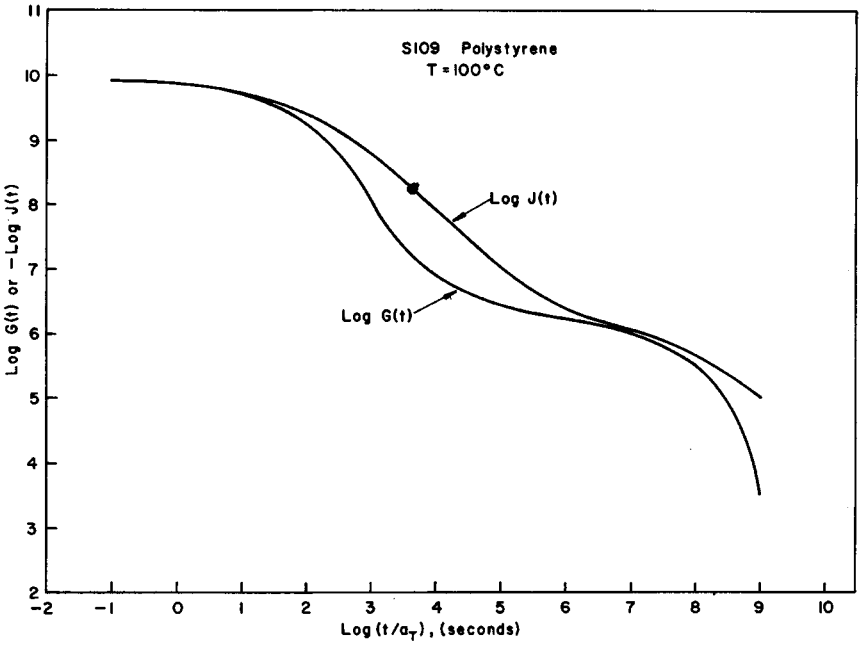

Fig. 5. Relaxation modulus from reference 7 and creep compliance calculated using 5 points per decade of logarithmic time for S109 polystyrene. $G(t)$ and $J(t)$ are in dynes/cm² and cm²/dyne, respectively.

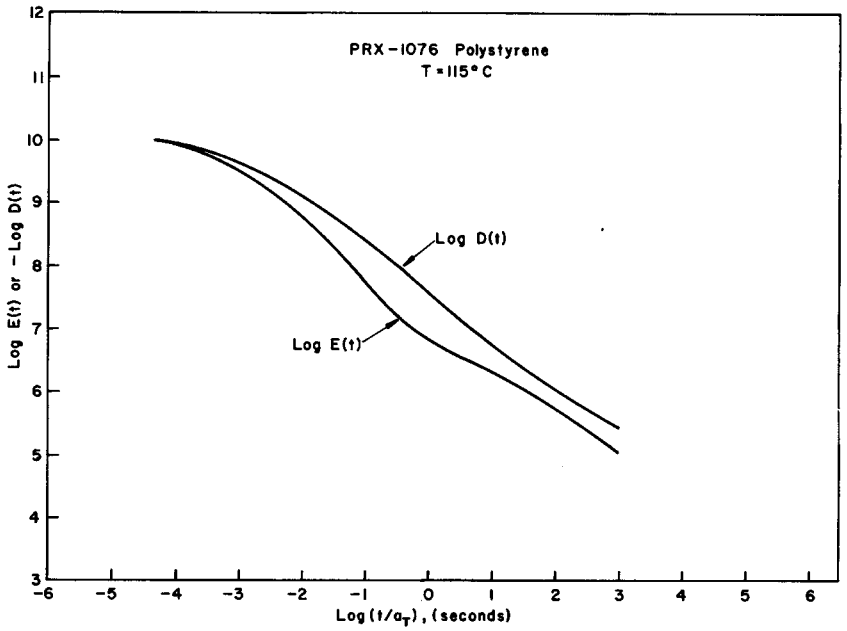

Fig. 6. Relaxation modulus and creep compliance from reference 8 for PRX-1076 polystyrene using 10 points per decade of logarithmic time. Units are same as in Fig. 5.

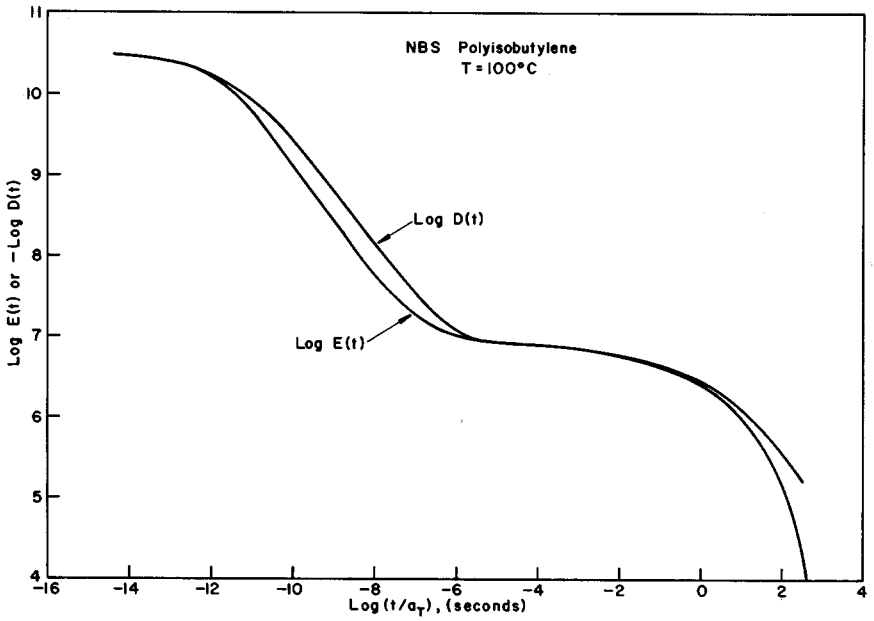

Fig. 7. Relaxation modulus and creep compliance for NBS polyisobutylene from reference 9 using 10 points per decade of logarithmic time. Units are same as in Fig. 5.

These samples range from the low molecular weight PRX-1076 to the rather high molecular weight NBS polyisobutylene. In all three cases, the moduli returned by eq. (30) from the compliance calculated by eq. (29) were well within 1% of the original data.

It must be noted that the polyisobutylene conversions were performed in two parts. The first was for the times between the points where

$$E(t) \cdot D(t) = 1 \tag{34}$$

at approximately log time = −14 and −4. The second was for all log times greater than −4. This procedure was made necessary by numerical errors in the calculation in a region of approximately constant modulus or compliance. This proved to be no serious fault. The restriction set by eq. (34) seems to be a necessary and sufficient condition for the exclusion of all the previous data as negligible, as long as $X(t(1))$ for the second calculation is taken as the plateau value. For example, in the second part of the polyisobutylene conversion, log $E(0)$ or $-\log D(0)$ would be approximately 6.90.

We offer a complete listing of the programs used in this paper to anyone upon request. They are written in Fortran IV language and were run on an IBM 360/91.

We have attempted to keep the names in the previous derivation consistent with those in the programs in order to reduce confusion. These

programs require approximately 40,000 locations of main core and have execution times of approximately 3 seconds for 100 points.

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