

A CURVE-FITTING PROGRAM TO STRESS RELAXATION DATA

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A computer program has been developed for the analysis of stress relaxation data using the method of successive residuals. This technique eliminates the use of graph paper and eye judgement for developing a multi-term exponential stress relaxation equation. This program has the potential to select best fit multi-term exponential equations to exponential decay data.

INTRODUCTION

Viscoelastic materials show a stress relaxation phenomenon which is one of the most important parameters in characterizing materials (Ferry 1961). In stress relaxation the test specimen is suddenly brought to a given strain, and the stress required to hold the deformation constant is measured as a function of time. The results are expressed in terms of a time-dependent modulus $E(t)$ in tension or compression, $G(t)$ in shear, or $K(t)$ in bulk compression. These parameters can be used either in direct form or in their reciprocal form called compliance in viscoelastic analyses.

One rheological model representing stress relaxation is the generalized Maxwell model as illustrated in Fig. 1. If this model is subjected to constant strain ϵ_0 at time $t = 0$, the total stress σ in the model is given by

$$\sigma = \sigma_1 + \sigma_2 + \sigma_3 + \dots + \sigma_n + \sigma_e \quad (1)$$

where σ_e is equilibrium stress.

The decrease in stress with time can be represented by

$$\sigma(t) = \epsilon_0 [E_{d1} e^{-t/\tau_1} + E_{d2} e^{-t/\tau_2} + \dots + E_{dn} e^{-t/\tau_n} + E_e] \quad (2)$$

where $\tau_1, \tau_2, \dots, \tau_n$ are relaxation times, τ_{rel} , corresponding to various elements in the model; E_0 is the initial modulus; E_d is the decay modulus ($E_0 - E_e$); and E_e is the equilibrium modulus.

To predict stress at any time, t , the stress relaxation curve must be represented by a mathematical expression depicting the behavior of the material under constant strain. The plot of the logarithm of stress versus time is generally nonlinear. It has been found that a three-term exponential equation is usually a reasonably good fit for practical purposes (Mohsenin 1978). Various graphical techniques outlined by Mohsenin (1978) and numerical analysis methods given by Moore (1974) can be used to express the relaxation curve in

terms of exponential functions. The most commonly used method is that of successive residuals. This method, however, is rather time consuming, and the accuracy using graphical technique depends upon personal judgement. It is the purpose of this study to develop a suitable computer program to be used to analyze the stress relaxation data by the method of successive residuals.

DESCRIPTION OF THE COMPUTER PROGRAM

If the stress relaxation is expressed in the general form of

$$\sigma(t) = \sigma_e + \sum_{n=1}^n \sigma_n e^{-t/\tau_n} \quad (3)$$

then the computer program begins by looking at either slope or change in stress values corresponding to equal time intervals in order to obtain the straight line portion of the log-stress versus time curve to compute σ_n and τ_n of Eq. 3 from the slope and ordinate intercept, respectively. The program takes the stress relaxation data and converts the stress or stress relaxation modulus into a logarithmic form. The semi-log curve is then divided into a large number of equal time segments. The cubic spline function (Erh 1972) is used to look at the incremental slopes or change in

stress values for equal time intervals. The spline function is also available in a subroutine form in the International, Mathematical and Statistical Library (IMSL) package. The incremental slope or change in stress values and time arrays are scanned backward to arrange them in a decreasing order of time. Equal incremental slope or change in stress values for constant time intervals will detect the straight line portion of the stress relaxation curve. The computer, however, performs very accurate analysis resulting in very large numbers of σ and τ . Since, for most practical purposes, three exponential functions are adequate for representing stress relaxation data, the problem is solved by taking the difference in the adjacent incremental slopes or change in stress values and comparing them with a very small value of tolerance. After obtaining the points for the straight line portion of the log-stress versus time curve, the data points are arranged in an increasing order of time, and the equation of the straight line portion is obtained by simple linear regression. The slope of the straight line portion gives time constant τ_1 and the intercept on the ordinate gives the coefficient of the exponential term σ_1 . The first residual is obtained by taking the difference between the original stress versus

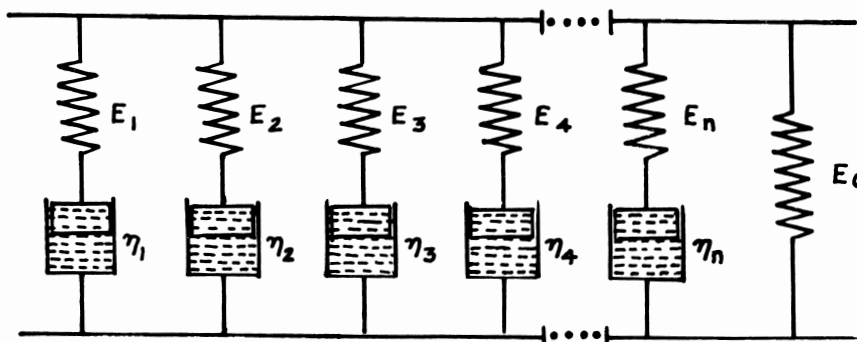


Figure 1. Generalized Maxwell model representation.

TABLE I. STRESS RELAXATION DATA FOR WHEAT DOUGH (CUNNINGHAM ET AL. 1953)

Time (S)	Tension (g)
0.0	710.0
1.0	560.0
2.0	487.0
4.0	420.0
6.0	383.0
8.0	355.0
10.0	334.0
12.0	321.0
14.0	309.0
16.0	298.0
18.0	288.0
20.0	280.0

time curve and the straight line portion extrapolated to the ordinate. This procedure was repeated two more times to obtain σ_2 and σ_3 , and τ_2 and τ_3 . The following steps describe the procedure in detail.

- (1) Read the data of stress relaxation.
- (2) Compute the natural logarithm of stress or stress relaxation modulus values.
- (3) Set the index value equal to the number of exponential terms required.
- (4) Set the values for tolerance.
- (5) Divide the time data into about 50 equal segments.
- (6) Use the spline procedure to compute the incremental slopes (DS) or change in stress values (DY) for equal time intervals.
- (7) Compute the difference between incremental slope (DIF) or change in stress values (DIFF) for equal time interval I and I + 1 as:

$$\begin{aligned} \text{DIF} &= \text{DS}(I + 1) - \text{DS}(I) \\ \text{DIFF} &= \text{DY}(I + 1) - \text{DY}(I) \end{aligned}$$

where DS = incremental slope, and DY = stress value.

- (8) Compare the difference (DIFF) with tolerance.
- (9) Take the points of log-stress and time for which DIFF or DIF is less than tolerance to obtain the points for the straight line portion of the log-stress versus time curve.

(10) Compute the values of σ and τ by simple linear regression.

(11) Compute the differences (STMD) between the original stress and the stress $N\sigma$ obtained from the straight line to obtain the first residual.

$$\text{STMD}(I) = \sigma(I) - N\sigma(I)$$

(12) If STMD is less than or equal to zero, then omit that value.

(13) Compute the natural logarithm of the STMD values.

(14) Repeat steps 4–11 two more times to obtain terms for the second and third exponentials.

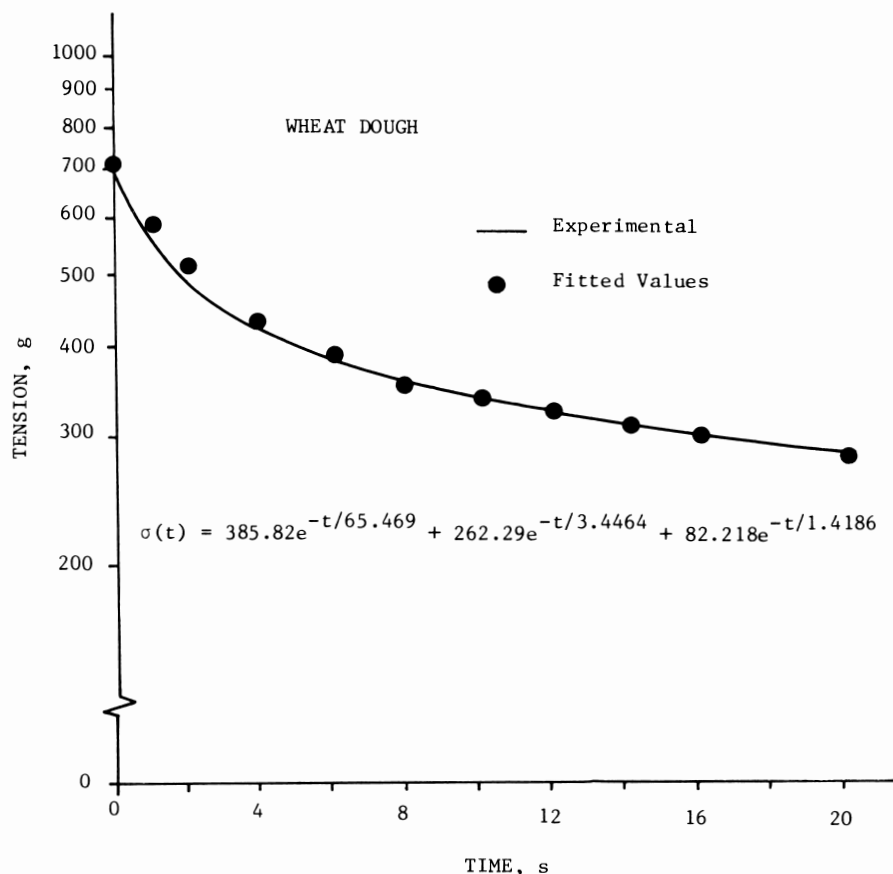


Figure 2. Comparison of experimental and computed values for stress relaxation $\sigma(t)$ for wheat dough. (Data from Cunningham et al. 1953.)

RESULTS AND DISCUSSION

The application of the method developed has been described by an illustrated example for wheat dough. The data for this example, given in Table I, were taken from Cunningham et al. (1953). The analysis was performed by assuming a zero value of equilibrium stress. The data representing the stress versus time relationship were divided into 50 equal time segments. With a tolerance value of 0.005, the program generated values of 385.82 and -65.469 for σ_1 and τ_1 , respectively. The corresponding stress values for the first residual are given in Table II. The repetition of the procedure resulted in values of 262.29, 82.218, -3.4464 and -1.4166 for σ_2 , σ_3 , τ_2 and τ_3 , respectively. The stresses associated with the second residual are also shown in Table II. The curve and equations developed from this analysis are shown in Fig. 2. Comparison with the experimental data yielded very good agreement with the fitted values, with a determination coefficient (r^2) of 0.991. Statistical analysis indicated no significant difference between the fitted values and experimental curve at the 0.05 level.

Some food materials do exhibit equilibrium stresses. In such cases this method

TABLE II. STRESS AND TIME DATA FOR THE FIRST AND SECOND RESIDUAL AS PREDICTED BY THE COMPUTER PROGRAM

First residual		Second residual	
Time (S)	Tension (g)	Time (S)	Tension (g)
0.0	344.20	0.0	81.89
0.41	275.60	0.36	46.99
0.82	219.50	0.72	18.85
1.63	149.80	2.15	16.32
2.86	99.26	2.87	15.19
3.67	79.45	3.22	13.49
4.90	65.02	3.94	9.30
5.71	48.62	4.30	7.27
6.53	39.70	4.66	5.45
7.35	31.85	5.02	3.83
8.57	21.94	5.37	2.44
9.39	16.81	5.73	1.30
10.20	13.22	6.09	0.43
11.43	10.36	6.45	0.17
12.65	8.19		
13.47	6.60		
14.69	4.48		
15.51	3.29		
16.73	1.68		
17.55	0.76		

was used by manipulating the equilibrium stress or modulus (σ_e or E_e) in $\sigma(t)$ or $E(t)$. Analysis performed on wheat dough with a value of 40 g for σ_e and a value of 0.005 for tolerance predicted the following equation.

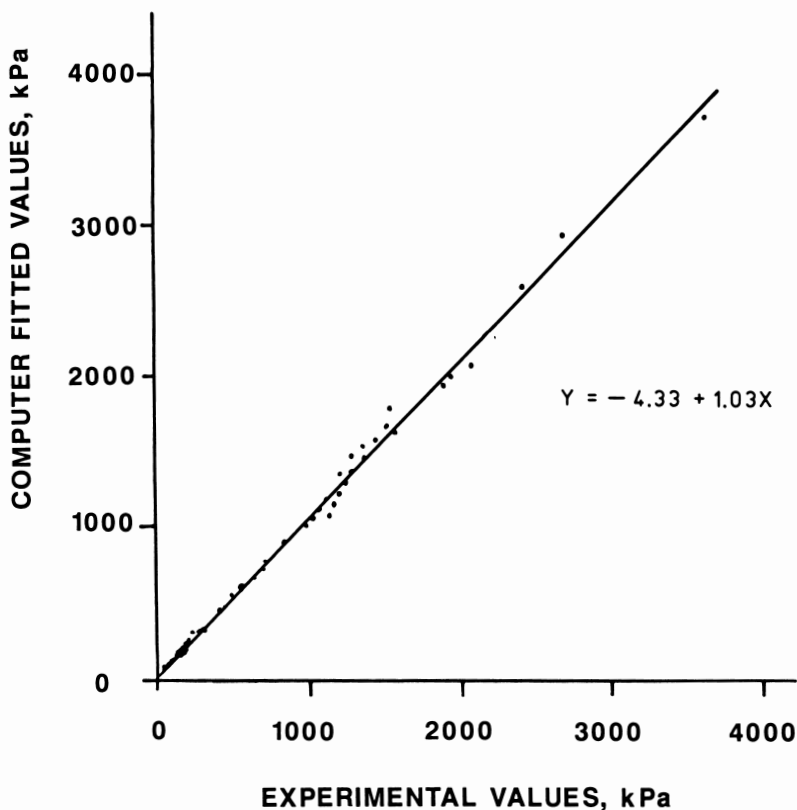


Figure 3. Comparison between the experimental and computer fitted values for stress relaxation for food materials.

$$\sigma(t) = 327.74e^{-\frac{t}{66.19}} + 258.86e^{-\frac{t}{3.37}} + 81.56e^{-\frac{t}{1.307}} + 40.0 \quad (4)$$

Comparison of this equation with the experimental curve yields a determination coefficient of 0.991. In this case, also, there was no significant difference between the fitted and experimental values at the 0.05 level.

To check the application further, this method was applied to stress relaxation data for bovine muscle, apple flesh and cheese. The experimental data reported by Morrow and Mohsenin (1969) for bovine muscle, Morrow et al. (1971) for apple flesh and Shama and Sherman (1973) for cheese were used. In all cases the fitted equation compared very well with the experimental data. The lowest determina-

tion coefficient of 0.984 between the fitted and experimental values was obtained for bovine muscle. To test the overall performance of this method the comparison was made between the pooled fitted and experimental values for all food materials reported earlier. The results presented in Fig. 3 show an excellent agreement with a determination coefficient of 0.996. This line was not significantly different from the equal value line at the 0.05 level. Comparison of this method with the graphical technique of stress relaxation given by Mohsenin (1978) also did not show any significant difference at the 0.05 level.

CONCLUSIONS

On the basis of the comparison made for different food materials, it was found that

the technique of fitting the computer curve to the stress relaxation data, based on the method of successive residuals developed in this study, is an easy and reliable method for determining the exponential functions representing given stress-relaxation data. This method can handle any number of exponential terms depending upon the precision and accuracy required. This method can also be used to obtain the best exponential curve fit by calculating the linear determination coefficient between the values obtained for a different number of exponential terms and the experimental data, comparing the fitted values with the experimental data, taking the one with the highest determination coefficient and not significantly different from the experimental data as the best fit curve. The method is simple, accurate and less time consuming.

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