

A Free Energy Functional for Thermorheologically Simple Materials

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With 3 Figures

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Summary — Zusammenfassung

A Free Energy Functional for Thermorheologically Simple Materials. A systematic procedure developed by COLEMAN for establishing thermodynamically consistent constitutive equations is used to develop the thermomechanical constitutive equations for the stress and dissipation functions for thermorheologically simple materials. A comparison is made with similar expressions developed using phenomenological model theory. The influence of thermorheologically simple behavior is illustrated in the solution of the problem of a solid rod undergoing torsional oscillations with temperature dependent properties.

Eine Darstellung der freien Energie thermorheologisch-einfacher Werkstoffe. Eine von COLEMAN entwickelte systematische Methode zur Aufstellung thermodynamisch konsistenter Werkstoffgleichungen wird zur Bestimmung der Werkstoffgleichungen für Spannungs- und Dissipationsfunktion thermorheologisch-einfacher Werkstoffe verwendet. Ein Vergleich mit ähnlichen Ausdrücken phänomenologischer Theorien wird durchgeführt. An Hand der Lösung des Problems eines Torsionsschwingers mit temperaturabhängigen Werkstoffeigenschaften wird der Einfluß des thermorheologisch-einfachen Verhaltens erläutert.

1. Introduction

The increasing use of viscoelastic materials in applications where significant amounts of heat may be generated due to thermomechanical coupling has created an interest in this phenomenon. The mathematical equations which model this behavior must be developed with the guidance of both the sciences of thermodynamics and mechanics since the displacement and thermal fields in boundary value problems which include heat generation are interrelated. As is often the case in describing material behavior, the forms of the constitutive equations which describe the thermomechanical behavior have been the objects of much discussion. The main concern in this area has been the appropriate form of the "dissipation function" for viscoelastic solids with temperature dependent properties.

The mathematical constitutive equation developments in the area of thermomechanical coupling in viscoelastic solids have mainly followed one of three basic approaches; the phenomenological model approach first expounded by STAVERMAN and SCHWARZL [1], the theory of irreversible thermodynamics described by BIOT [2], or the concepts of COLEMAN [3] which are based upon a recognition of how the state variables are related in a topological space. Although

these three approaches are very different in concept, they lead to very similar results [4]. The approach described by COLEMAN [5] appears to be the more easily acceptable from a rational mathematical standpoint although BIOT's [2] developments have been more widely used to the current time. In the developments described here, attention will be restricted mainly to the results of Coleman's work.

Summaries of tentative forms for the governing thermomechanical equations have been presented by HUNTER [6] and PARKUS [7] while significant applications of Biot's theory have been made by SCHAPERY [8], [9]. CHRISTENSEN and NAGHDI [10] have derived an expression for the dissipation function for a particular class of non-isothermal viscoelastic solids which does not include "thermorheologically simple" materials and HUANG [11] has postulated an expression for the dissipation function which employs the concepts used by BIOT [2].

A thermodynamically consistent development of the thermomechanical constitutive equations for "thermorheologically simple" materials seems to be lacking. The purpose of this paper is to demonstrate the usefulness of Coleman's procedure for generating specific constitutive relations by developing the thermomechanical equations for thermorheologically simple viscoelastic materials and to compare the form of the thermomechanical equations with other results based upon a phenomenological model theory. Also, the influence of temperature dependent viscoelastic properties on the heat generated is illustrated in a boundary value problem.

2. Thermomechanical Equations for Thermorheologically Simple Materials

In what follows, the basic constitutive relations for thermorheologically simple materials are developed by using the operators defined by COLEMAN. Details of the development are included to demonstrate the general technique. The method of approach is as follows; an assumption is made for the form of the free energy functional and the appropriate operators applied to obtain the constitutive expressions for the stresses, entropy, and internal dissipation. If the derived stress equation agrees with the commonly accepted stress expressions [12], the expressions for entropy and internal dissipation are assumed valid. The development is carried out assuming the spatial gradient of the temperature is small. The notation employed is that of COLEMAN [3].

Recall that the deviatoric and dilatational stress constitutive equations for a thermorheologically simple material are expressed, respectively, as [12]

$$\hat{s}_{ij}(\mathbf{x}, \xi) = \int_0^{\xi} 2G(\xi - \xi') \frac{\partial \hat{e}_{ij}(\mathbf{x}, \xi')}{\partial \xi'} d\xi', \quad (1a)$$

and

$$\hat{\sigma}(\mathbf{x}, \xi) = \int_0^{\xi} 3K(\xi - \xi') \frac{\partial [\hat{\gamma}(\mathbf{x}, \xi') - \alpha_0 \hat{T}(\mathbf{x}, \xi')]}{\partial \xi'} d\xi', \quad (1b)$$

where the \hat{s}_{ij} and \hat{e}_{ij} are the stress and strain deviators defined as

$$\hat{s}_{ij} = \hat{\sigma}_{ij} - \frac{1}{3} \delta_{ij} \hat{\sigma}_{kk} \quad \text{and} \quad \hat{e}_{ij} = \hat{\gamma}_{ij} - \frac{1}{3} \delta_{ij} \hat{\gamma}_{kk} \quad (2)$$

and $\hat{\sigma}_{ij}$ and $\hat{\gamma}_{ij}$ are components of the stress and strain tensors and δ_{ij} denotes the Kronecker delta. The mean stress and strain are defined, respectively, as

$$\hat{\sigma} = \frac{1}{3} \sigma_{kk} \quad \text{and} \quad \hat{\gamma} = \frac{1}{3} \gamma_{kk}. \tag{3}$$

In (1), $G(t)$ and $K(t)$ are the isothermal shear and bulk relaxation moduli, respectively, \hat{T} is a pseudo temperature defined as

$$\hat{T}(\mathbf{x}, \xi) = \frac{1}{\alpha_0} \int_0^{T(\mathbf{x}, \xi)} \alpha(T') dT', \quad \alpha_0 = \alpha(T_0) \tag{4}$$

where $\alpha(T)$ is the temperature dependent linear coefficient of thermal expansion and T_0 is a reference temperature. The notation \mathbf{x} in (1) denotes the triplet of spatial coordinates (x_1, x_2, x_3) and ξ is a reduced time defined in terms of real time t as

$$\xi(\mathbf{x}, t) = \int_0^t \varphi[T(\mathbf{x}, \tau)] d\tau \tag{5}$$

where $\varphi[T(\mathbf{x}, t)]$ is termed the shift factor [12]. The symbol $\hat{s}_{ij}(\mathbf{x}, \xi)$ is used to denote the function resulting from a mapping of the (\mathbf{x}, t) space onto the (\mathbf{x}, ξ) space. $\hat{s}_{ij}(\mathbf{x}, \xi)$ is defined as

$$\hat{s}_{ij}(\mathbf{x}, \xi) \equiv s_{ij}(\mathbf{x}, t) = s_{ij}[\mathbf{x}, g(\xi)] \tag{6}$$

and where $g(\xi)$ is the inverse of (5). A similar argument holds for other quantities crowned with a caret symbol.

Utilizing rational mechanics concepts, the basic constitutive assumption for a material may be expressed in the form of a free energy functional which for a thermorheologically simple material is assumed to have the form¹

$$\begin{aligned} \rho \hat{\Psi} = & \Psi_0 + \int_0^\xi D_{ij}(\xi - \xi') \frac{\partial \hat{\gamma}_{ij}}{\partial \xi'} d\xi' - \int_0^\xi f(\xi - \xi') \frac{\partial \hat{T}}{\partial \xi'} d\xi' \\ & + \frac{1}{6} \int_0^\xi \int_0^\xi [3K(\xi - \xi', \xi - \xi'') - 2G(\xi - \xi', \xi - \xi'')] \frac{\partial \hat{\gamma}_{ij}}{\partial \xi'} \frac{\partial \hat{\gamma}_{kk}}{\partial \xi''} d\xi' d\xi'' \\ & + \frac{1}{2} \int_0^\xi \int_0^\xi 2G(\xi - \xi', \xi - \xi'') \frac{\partial \hat{\gamma}_{ij}}{\partial \xi'} \frac{\partial \hat{\gamma}_{ij}}{\partial \xi''} d\xi' d\xi'' \\ & - \int_0^\xi \int_0^\xi 3\alpha K(\xi - \xi', \xi - \xi'') \frac{\partial \hat{\gamma}_{kk}}{\partial \xi'} \frac{\partial \hat{T}}{\partial \xi''} d\xi' d\xi'' \\ & - \frac{1}{2} \int_0^\xi \int_0^\xi m(\xi - \xi', \xi - \xi'') \frac{\partial \hat{T}}{\partial \xi'} \frac{\partial \hat{T}}{\partial \xi''} d\xi' d\xi'', \end{aligned} \tag{7}$$

¹ This functional represents an extension of the functional expansion described by CHRISTENSEN and NAGHDI [10].

where, by recalling (6), it is understood that

$$\rho \hat{\Psi}(\mathbf{x}, \xi) \equiv \rho \Psi(\mathbf{x}, t) = \rho \Psi[\mathbf{x}, g(\xi)], \quad (8)$$

where $\Psi(\mathbf{x}, t)$ is the free energy density functional for an isothermal viscoelastic material.

The stress tensor can be obtained from the free energy functional (7) by application of the operator $D_{\hat{\mathbf{F}}}$ as described by COLEMAN [3] where \mathbf{F} is the deformation gradient. For simplicity, consider only the components of the stress and strain tensors. For this case the stress operator equation (3) reduces to

$$\hat{\sigma}_{ij} = \rho D_{\hat{\mathbf{F}}_{ij}} \hat{\Psi}[\hat{\mathbf{F}}^\xi(s), \hat{T}^\xi(s)] \quad (9)$$

where the operator $D_{\hat{\mathbf{F}}_{ij}}$ is defined as²

$$D_{\hat{\mathbf{F}}_{ij}} \hat{\Psi}[\hat{\mathbf{F}}^\xi(s), \hat{T}^\xi(s)] = \frac{\partial}{\partial \hat{\mathbf{F}}_{ij}} \hat{\Psi}[\hat{\mathbf{F}}_r^\xi(s), \hat{T}_r^\xi(s); \hat{\mathbf{F}}, \hat{T}]. \quad (10)$$

As seen in (10), if the strain energy functional is expressed in terms of the past histories of the deformation gradient and temperature, the operator $D_{\hat{\mathbf{F}}}$ becomes simply the partial derivative of the free energy functional with respect to the present values of the deformation gradient tensor components $\hat{\mathbf{F}}_{ij}$.

To apply the operator $D_{\hat{\mathbf{F}}_{ij}}$, the functional $\hat{\Psi}$ in (7) must be expressed in terms of the past history of the deformation gradient. The infinitesimal strain tensor components $\hat{\gamma}_{ij}$ are related to the components of the deformation tensor $\hat{\mathbf{F}}_{ij}$ by the expression

$$\hat{\gamma}_{ij} = \frac{1}{2} (\hat{\mathbf{F}}_{ij} + \hat{\mathbf{F}}_{ji} - 2\delta_{ij}). \quad (11)$$

The integrals in (7) may be transformed, by integrating by parts, into integrals involving the derivatives of the kernel functions. Since the partial derivatives in (10) are taken with respect to the present values of $\hat{\mathbf{F}}$, the integral terms in (7) which involve the histories will not be converted to expressions in terms of $\hat{\mathbf{F}}$ but instead will be left in terms of the strain components which are possibly more familiar measures of deformation. Carrying out these transformations on (7) gives

$$\begin{aligned} \rho \hat{\Psi} = & \Psi_0 + D_{ij}(0) (\hat{\mathbf{F}}_{ij} - \delta_{ij}) - \int_0^\xi \frac{\partial}{\partial \xi'} D_{ij}(\xi') \hat{\gamma}_{ij}^\xi(\xi') d\xi' - f(0) \hat{T}(\xi) \\ & + \int_0^\xi \frac{\partial}{\partial \xi'} f(\xi') \hat{T}^\xi(\xi') d\xi' \\ & + \frac{1}{6} \left\{ M(0, 0) (\hat{\mathbf{F}}_{ii} - 3) (\hat{\mathbf{F}}_{jj} - 3) - 2(\hat{\mathbf{F}}_{ii} - 3) \int_0^\xi \frac{\partial}{\partial \xi'} M(0, \xi') \hat{\gamma}_{jj}^\xi(\xi') d\xi' \right. \\ & \left. + \int_0^\xi \int_0^\xi \frac{\partial^2}{\partial \xi' \partial \xi''} M(\xi', \xi'') \hat{\gamma}_{ii}^\xi(\xi') \hat{\gamma}_{jj}^\xi(\xi'') d\xi' d\xi'' \right\} \end{aligned}$$

² See equation (3.8a) in COLEMAN and GURTIN [15].

$$\begin{aligned}
 & + \frac{1}{2} \left\{ \frac{1}{2} G(0, 0) (\hat{F}_{ij} + \hat{F}_{ji} - 2\delta_{ij}) (\hat{F}_{ij} + \hat{F}_{ji} - 2\delta_{ij}) \right. \\
 & \quad - 2(\hat{F}_{ij} - \delta_{ij}) \int_0^\xi \frac{\partial}{\partial \xi'} 2G(0, \xi') \hat{\gamma}_{ij}^\xi(\xi') d\xi' \\
 & \quad \left. + \int_0^\xi \int_0^\xi \frac{\partial^2}{\partial \xi' \partial \xi''} 2G(\xi', \xi'') \hat{\gamma}_{ij}^\xi(\xi') \hat{\gamma}_{ij}^\xi(\xi'') d\xi' d\xi'' \right\} \\
 & - \left\{ 3\alpha K(0, 0) \hat{T}(\hat{F}_{ij} - 3) - (\hat{F}_{ij} - 3) \int_0^\xi \frac{\partial}{\partial \xi'} 3\alpha K(0, \xi') \hat{T}^\xi(\xi') d\xi' \right. \\
 & \quad - \hat{T} \int_0^\xi \frac{\partial}{\partial \xi'} 3\alpha K(\xi', 0) \hat{\gamma}_{kk}^\xi(\xi') d\xi' \\
 & \quad \left. + \int_0^\xi \int_0^\xi \frac{\partial^2}{\partial \xi' \partial \xi''} 3\alpha K(\xi', \xi'') \hat{T}^\xi(\xi') \hat{T}^\xi(\xi'') d\xi' d\xi'' \right\} \\
 & - \frac{1}{2} \left\{ m(0, 0) \hat{T} \hat{T} - 2\hat{T} \int_0^\xi \frac{\partial}{\partial \xi'} m(0, \xi') \hat{T}^\xi(\xi') d\xi' \right. \\
 & \quad \left. + \int_0^\xi \int_0^\xi \frac{\partial^2}{\partial \xi' \partial \xi''} m(\xi', \xi'') \hat{T}^\xi(\xi') \hat{T}^\xi(\xi'') d\xi' d\xi'' \right\}.
 \end{aligned} \tag{12}$$

In arriving at (12), it is assumed that all kernels are symmetric with respect to their double arguments and that the initial values of the temperature and strains are zero. Also, kernel $M(\xi', \xi'')$ has been defined, for brevity, to be

$$M(\xi', \xi'') = 3K(\xi', \xi'') - 2G(\xi', \xi''). \tag{13}$$

Applying the operator defined in (10) to (12) gives

$$\begin{aligned}
 \hat{\sigma}_{ij} & = D_{ij}(0) + \frac{1}{3} \delta_{ij} M(0, 0) \hat{\gamma}_{kk}(\xi) - \frac{1}{3} \delta_{ij} \int_0^\xi \frac{\partial}{\partial \xi} M(0, \xi') \hat{\gamma}_{kk}^\xi(\xi') d\xi' \\
 & + 2G(0, 0) \hat{\gamma}_{ij}(\xi) - \int_0^\xi \frac{\partial}{\partial \xi'} 2G(0, \xi') \hat{\gamma}_{ij}^\xi(\xi') d\xi' - \delta_{ij} 3\alpha K(0, 0) \hat{T}(\xi) \\
 & + \delta_{ij} \int_0^\xi \frac{\partial}{\partial \xi'} 3\alpha K(0, \xi') \hat{T}^\xi(\xi') d\xi'.
 \end{aligned} \tag{14}$$

Assuming the initial stress is zero, expressing all terms as a function of the kernels $K(\xi)$ and $G(\xi)$, where $K(0, \xi)$ and $G(0, \xi)$ are defined, respectively, as $K(\xi)$ and $G(\xi)$, and integrating by parts allows (14) to be expressed as

$$\begin{aligned} \delta_{ij} = & \int_0^{\xi} 2G(\xi - \xi') \frac{\partial \hat{\gamma}_{ij}}{\partial \xi'} d\xi' + \frac{1}{3} \delta_{ij} \int_0^{\xi} [3K(\xi - \xi') - 2G(\xi - \xi')] \frac{\partial \hat{\gamma}_{kk}}{\partial \xi'} d\xi' \\ & - \delta_{ij} \int_0^{\xi} 3\alpha K(\xi - \xi') \frac{\partial \hat{T}}{\partial \xi'} d\xi' \end{aligned} \quad (15)$$

which is the stress equation for a thermorheologically simple material which results if (1) and (2) are combined. It is concluded that (7) must be a correct form for the free energy functional for a thermorheologically simple material since (15) agrees with the stress equations known a priori.

In a similar manner, the expression for the entropy can now be derived from the free energy functional by application of the operator $D_{\hat{T}}$ which has been presented by COLEMAN and GURTIN [14] (Eqn. (3.86)) in the form

$$D_{\hat{T}} \hat{\Psi}(\hat{\mathbf{F}}^{\xi}, \hat{T}^{\xi}) = \frac{\partial}{\partial \hat{T}} \hat{\Psi}(\hat{\mathbf{F}}_r^{\xi}, \hat{T}_r^{\xi}; \hat{\mathbf{F}}, \hat{T}). \quad (16)$$

Application of this operator to the free energy functional (7) and subsequent integration by parts results in the expression³

$$\rho \hat{\eta} = \int_0^{\xi} 3\alpha K(\xi - \xi') \frac{\partial \hat{\gamma}_{kk}}{\partial \xi'} d\xi' + \int_0^{\xi} m(\xi - \xi') \frac{\partial \hat{T}}{\partial \xi'} d\xi', \quad (17)$$

where $f(0)$ has been assumed zero to satisfy the requirement of zero initial conditions.

Finally, consider the expression for the internal dissipation σ^* which may also be obtained from the free energy functional. The internal dissipation may be expressed as

$$\sigma^*(t) = \frac{1}{T(t)} \left[\frac{1}{\rho} \sigma_{ij} \dot{\gamma}_{ij} - \eta \dot{T} - \dot{\Psi} \right]. \quad (18)$$

The quantity $\sigma^*(t)$ in (18) is a rate of internal dissipation in terms of real time; it can be related to the dissipation in the reduced time variable by the relation⁴

$$\sigma^*(t) = \delta^*(\xi) \frac{d\xi}{dt} = \delta^*(\xi) \varphi(T). \quad (19)$$

By transforming all of the terms in (18) to reduced time, the internal dissipation function becomes

$$\delta^* = \frac{1}{\hat{T}} \left[\frac{1}{\rho} \delta_{ij} \hat{\gamma}_{ij} - \hat{\eta} \hat{T} - \hat{\Psi} \right] \quad (20a)$$

³ This agrees with the entropy expression determined by CHRISTENSEN and NAGHDI [10] who used a different method of derivation, when specialized to the isothermal case.

⁴ The function $\sigma^*(t)$ employed by COLEMAN [3] is related to the dissipation function \mathcal{A} employed by CHRISTENSEN and NAGHDI [10] by the relation $\rho T \sigma^* = \mathcal{A}$.

where

$$\dot{f} = \frac{d\hat{f}(\xi)}{d\xi} = \frac{1}{\varphi(T)} \frac{df(t)}{dt}. \tag{20b}$$

Since the expressions for δ_{ij} and $\hat{\eta}$ have already been developed in (15) and (17), it remains to calculate $\hat{\Psi}$ and to substitute into (20a) along with expressions for the stress and entropy. Performing these operations gives the expression for the dissipation function as

$$\begin{aligned} \rho \hat{T}(\xi) \delta^*(\xi) = & -\frac{1}{6} \int_0^\xi \int_0^\xi \frac{\partial}{\partial \xi} [3K(\xi - \xi', \xi - \xi'')] \\ & - 2G(\xi - \xi', \xi - \xi'')] \frac{\partial \hat{\gamma}_{ii}}{\partial \xi'} \frac{\partial \hat{\gamma}_{ij}}{\partial \xi''} d\xi' d\xi'' \\ & - \frac{1}{2} \int_0^\xi \int_0^\xi \frac{\partial}{\partial \xi} [2G(\xi - \xi', \xi - \xi'')] \frac{\partial \hat{\gamma}_{ij}}{\partial \xi'} \frac{\partial \hat{\gamma}_{ij}}{\partial \xi''} d\xi' d\xi'' \\ & + \int_0^\xi \int_0^\xi \frac{\partial}{\partial \xi} [3\alpha K(\xi - \xi', \xi - \xi'')] \frac{\partial \hat{\gamma}_{kk}}{\partial \xi'} \frac{\partial \hat{T}}{\partial \xi''} d\xi' d\xi'' \\ & + \frac{1}{2} \int_0^\xi \int_0^\xi \frac{\partial}{\partial \xi} [m(\xi - \xi', \xi - \xi'')] \frac{\partial \hat{T}}{\partial \xi'} \frac{\partial \hat{T}}{\partial \xi''} d\xi' d\xi''. \end{aligned} \tag{21}$$

The linear integral terms which would normally appear in (21) have been shown by CHRISTENSEN and NAGHDI [10] to be zero. With these developments the energy equation for this material can be expressed as

$$-\rho \hat{T} \dot{\eta} + \rho \hat{r} + \rho \hat{T} \delta^* = \hat{q}_{i,i}. \tag{22}$$

If Fourier's law of heat conduction is assumed applicable and (17) and (21) substituted into (22), the energy equation, expressed in reduced time, becomes

$$\begin{aligned} k \hat{T}_{,ii} = & m(0) \hat{T} \dot{T} + 3\alpha K(0) \hat{T} \hat{\gamma}_{kk} - \rho r \\ & + \frac{1}{6} \int_0^\xi \int_0^\xi \frac{\partial}{\partial \xi} [3K(\xi - \xi', \xi - \xi'')] \\ & - 2G(\xi - \xi', \xi - \xi'')] \frac{\partial \hat{\gamma}_{ii}}{\partial \xi'} \frac{\partial \hat{\gamma}_{kk}}{\partial \xi''} d\xi' d\xi'' \\ & + \frac{1}{2} \int_0^\xi \int_0^\xi \frac{\partial}{\partial \xi} [2G(\xi - \xi', \xi - \xi'')] \frac{\partial \hat{\gamma}_{ij}}{\partial \xi'} \frac{\partial \hat{\gamma}_{ij}}{\partial \xi''} d\xi' d\xi'' \\ & - \int_0^\xi \int_0^\xi \frac{\partial}{\partial \xi} [3\alpha K(\xi - \xi', \xi - \xi'')] \frac{\partial \hat{\gamma}_{kk}}{\partial \xi'} \frac{\partial \hat{T}}{\partial \xi''} d\xi' d\xi'' \\ & - \frac{1}{2} \int_0^\xi \int_0^\xi \frac{\partial}{\partial \xi} [m(\xi - \xi', \xi - \xi'')] \frac{\partial \hat{T}}{\partial \xi'} \frac{\partial T}{\partial \xi''} d\xi' d\xi''. \end{aligned} \tag{23}$$

In solving boundary value problems, it is desirable to have the energy equation expressed in terms of real time. Transforming (23) to the real time variable gives the energy equation in the form

$$\begin{aligned}
 kT_{,ii} = m(0)T\dot{T} + 3\alpha K(0)T\dot{\gamma}_{kk} - \rho r \\
 + \frac{1}{6} \int_0^t \int_0^t \frac{\partial}{\partial t} [3K(\xi - \xi', \xi - \xi'') \\
 - 2G(\xi - \xi', \xi - \xi'')] \frac{\partial \gamma_{ii}}{\partial t} \frac{\partial \gamma_{kk}}{\partial t'} dt' dt'' \\
 + \frac{1}{2} \int_0^t \int_0^t \frac{\partial}{\partial t} [2G(\xi - \xi', \xi - \xi'')] \frac{\partial \gamma_{ij}}{\partial t'} \frac{\partial \gamma_{ij}}{\partial t''} dt' dt'' \\
 - \int_0^t \int_0^t \frac{\partial}{\partial t} [3\alpha K(\xi - \xi', \xi - \xi'')] \frac{\partial \gamma_{kk}}{\partial t'} \frac{\partial T}{\partial t''} dt' dt'' \\
 - \frac{1}{2} \int_0^t \int_0^t \frac{\partial}{\partial t} [m(\xi - \xi', \xi - \xi'')] \frac{\partial T}{\partial t'} \frac{\partial T}{\partial t''} dt' dt''.
 \end{aligned} \tag{24}$$

3. Comparison of Theoretical Developments

The energy equation developed as stated in (24) applies for thermorheologically simple materials. Other statements of this equation have appeared in the literature [1], [2], [6], [7] and it seems worthwhile to compare the present results with those obtained previously. Recall that the energy equation for a linear elastic material is generally of the form

$$kT_{,ii} = \rho c \dot{T} + 3\alpha K T \dot{\gamma}_{kk} - \rho r \tag{25}$$

where the second term on the right hand side of (25) is due to thermomechanical coupling. By comparing (25) and (24) it is recognized that the first three terms of the viscoelastic energy equation are equivalent to the elastic energy equation. The only difference being the coefficient of the \dot{T} term which has been redefined in terms of a specific heat quantity which linearizes that term. In (25) the temperature variable T in the thermomechanical coupling term is often taken to be a constant reference temperature and thereby further simplifies the equation. If the first three terms of the viscoelastic energy equation (24) correspond to an elastic material, it is apparent that the remainder of the terms are contributions from the viscoelastic effect. Consequently, it is incorrect to refer to the magnitude of the thermomechanical coupling term in (25) when describing the dissipative character of viscoelastic materials.

HUNTER [6] and PARKUS [7] have both presented tentative forms of the energy equation for thermorheologically simple solids which were derived by considering spring dashpot models. It is not clear that manipulations with such

models satisfies the principles of irreversible thermodynamics. The energy equation (24) represents a slightly more general form than those of HUNTER [6] and PARKUS [7] but agrees in concept. The arguments of Hunter's [6] kernel functions are of the form $(2\xi - \xi' - \xi'')$ instead of $(\xi - \xi', \xi - \xi'')$ which suggests an exponential function kernel must be used in the phenomenological model equations. Since the bulk viscoelastic behavior of most polymers is small, these terms are not thought to have much effect. Furthermore, for the approaches of BIOT [2], COLEMAN [3], and STAVERMAN and SCHWARZL [1] to be exactly the same, the kernel function $m(t)$ in (24) must be defined as

$$m(t) = -9\alpha^2 K(t) \tag{26}$$

where $K(t)$ is the bulk modulus. If this is correct, then the terms having $m(t)$ as a kernel will probably be small for most polymers.

4. Torsional Oscillations of a Solid Cylinder

To demonstrate the influence of thermorheologically simple behavior on the heat generation phenomenon, consider a finite length cylinder of radius a and length l undergoing cyclic torsional oscillations as shown in Fig. 1. For the special

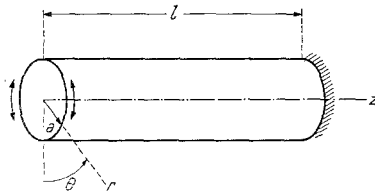


Fig. 1. Circular cylinder subjected to torsional oscillations

case when the deformations are cyclic, the dissipation function assumes a special form and it becomes convenient to work with a cycle-averaged dissipation function defined as

$$\bar{A} = \frac{\omega}{2\pi} \int_t^{t+\frac{2\pi}{\omega}} \sigma_{ij} \dot{\gamma}_{ij} dt' \tag{26}$$

where ω is the frequency of oscillation. The expression (26) is consistent with the previous definition for the dissipation function in (18) if it is assumed that the heat flux or heat generation is sufficiently low so that the term $\eta \dot{T}$ can be ignored and if it is realized the net energy stored per cycle is zero such that $\dot{\Psi}$ averaged over a cycle is zero. Using (26) the cycle-averaged energy equation (24) for the cylindrical geometry in Fig. 1, takes the form

$$k \left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2} \right) = \rho c_v \frac{\partial T}{\partial t} - \bar{A} \tag{27}$$

where the term ρr has been assumed zero. If one end of the circular rod is assumed fixed and the other twisted with a periodic motion, shearing stresses and strains are induced in the cylinder⁵. If the cylinder is oscillated at a frequency below the fundamental frequency of the system, inertia effects may be ignored and the displacements and strains determined simply from a knowledge of the imposed displacement boundary conditions. Specifically, if one end of the rod is subjected to the displacement

$$\theta(t) = \theta_0 \sin \omega t, \quad (27)$$

then, assuming plane sections remain plane, the only non-zero strain component is the component $\gamma_{\theta z}$, which can be assumed constant along the length of the cylinder and, consequently, can be expressed as

$$\gamma_{\theta z} = \left(\frac{\theta_0 r}{2l} \right) \sin \omega t, \quad (28)$$

where θ_0 is the maximum angle of twist of the rod.

Since the dilatation $\gamma = \frac{1}{3} \gamma_{ii}$ is zero for this case, the dissipation function contained in (24) reduces to

$$A(r, t) = \int_0^t \int_0^t 2 \frac{\partial}{\partial t} [2G(2\xi - \xi' - \xi'')] \frac{\partial \gamma_{\theta z}}{\partial t'} \frac{\partial \gamma_{\theta z}}{\partial t''} dt' dt''. \quad (29)$$

Because the strain is defined precisely in terms of the prescribed displacements, the dissipation function (29) becomes simply a prescribed heat generation term in the energy equation (27) and reduces the analysis to the problem of solving the heat conduction equation with a prescribed heat generation term which depends on time, temperature, and spatial coordinates. The relaxation modulus in (29) and, hence, the dissipation function itself depend on the local current value of the temperature. If the shear relaxation modulus is assumed to have the form

$$G(t) = \sum_{i=1}^n G_i e^{-\frac{t}{\tau_i}} \quad (30)$$

where the G_i and τ_i are material constants, the dissipation function can be expressed as

$$A(r, t) = -\varphi(T) \omega^2 \left[\frac{\theta_0 r}{2l} \right]^2 2 \sum_{i=1}^n \frac{G_i}{\tau_i} e^{-\frac{2\xi}{\tau_i}} \left[\int_0^t e^{\frac{\xi'}{\tau_i}} \cos \omega t' dt' \right]^2, \quad (31)$$

where $\varphi(T)$ is the shift factor and ξ the reduced time as defined in (5).

Due to the complicated form of the reduced time, the procedure for evaluating the dissipation function is not clear. For example, the WLF form of the shift

⁵ Although normal stresses and strains are present also, they are neglected in this analysis due to their smallness in comparison with the shearing stresses and strains.

factor [16] has been used extensively for amorphous polymers. This relation is of the form

$$\log_{10} \varphi [T(x, t)] = K_1 - \frac{K_2 [T(x, t) - T_s]}{K_3 + [T(x, t) - T_s]}, \quad (32)$$

where K_1 , K_2 , and K_3 and T_s are material constants determined by curve-fitting experimental data. Since the reduced time involves the temperature history, it is apparent what difficulties exist in evaluating the integrals in the dissipation function.

If we consider the special isothermal case then $\varphi = 1$ and $\xi = t$, the expression for the cycle-averaged dissipation function (26), becomes

$$\bar{A}(r) = \frac{1}{2} \left[\frac{\theta_0 r}{l} \right]^2 \omega G''(\omega) \quad (33)$$

where $G''(\omega)$ is the shear loss modulus.

Returning to consideration of the nonisothermal thermorheologically simple expression for the dissipation function, it should be noted that an expression of the form⁶

$$\bar{A}(r) \approx \frac{1}{2} \left[\frac{\theta_0 r}{l} \right]^2 \omega G'' \left[\frac{\omega}{\varphi(T)} \right] \quad (34)$$

has been used quite commonly as the expression for the thermorheologically dissipation function [9], [17]. Use of this equation is equivalent to the approximation

$$\xi(x, t) - \xi(x, t') = \varphi [T(x, t)] (t - t') \quad (35)$$

in the expression for the dissipation function (19). This approximation results in the dissipation function being overestimated and, consequently, too much heat being produced for a given oscillation. However, for purposes of comparison, the form of the dissipation function expressed in (34) was used in the analysis described here for the thermorheologically simple case.

The finite element method has proven to be a powerful numerical technique for solving a variety of field problems including structural analysis, seepage flow, heat conduction, and dynamic material response [18] problems. It appears to be a much more useful technique for solving boundary value problems which include complex material response and complex geometrical configurations than such classical techniques as integral transform methods.

Implementation of the finite element method can be viewed as an extension of the Ritz technique in which determination of a function which minimizes the functional [18]

$$\Gamma(T, \dot{T}) = \int_v \left[\frac{1}{2} \nabla T \cdot \mathbf{k} \nabla T + \rho c T \dot{T} - \Lambda T \right] dv - \int_s \mathbf{n} \cdot \mathbf{q} T ds \quad (36)$$

⁶ The shift factor φ used here is that described by MORLAND and LEE [12] which is the reciprocal of the quantity α_T used elsewhere [9], [17].

can be shown to be equivalent to solving the heat conduction equation

$$\nabla \cdot \mathbf{k} \nabla T = \rho c \dot{T} - A, \quad (37)$$

which is the Euler equation for this functional. In (36), ∇ denotes the del operator, \mathbf{k} the conductivity matrix, and A the dissipation function.

The finite element method was used to obtain a solution to the energy equation (27) for the circular cylindrical geometry described in Fig. 1 undergoing torsional oscillations. To provide a check on the accuracy of the solution technique, a problem considered by TAUCHERT [19] was solved which did not include temperature dependent viscoelastic material properties and which considered the cylindrical surface of the rod to be insulated and both ends of the rod to be maintained at a constant temperature T .

Since, in this special case, the dissipation function is of the form expressed in (33), which is independent of time, the energy equation (27) can be put into a dimensionless form which allows the temperature to be normalized with respect to the magnitude of the forcing function. A comparison of the finite element results and Tauchert's [19] Laplace transform results are shown in Fig. 2. The

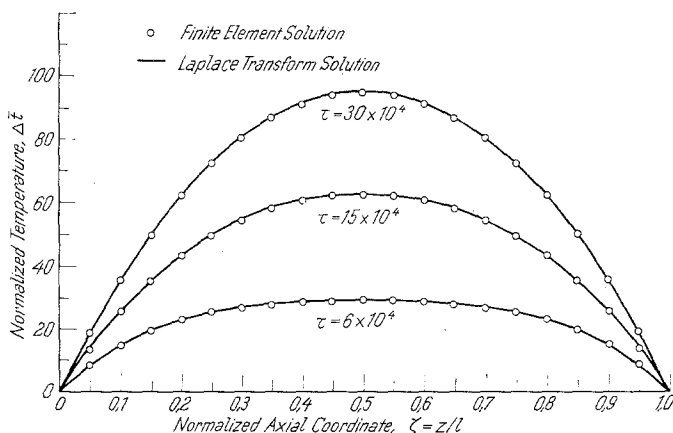


Fig. 2. Temperature at outer surface of cylinder

notation $\Delta \bar{T}$ is used to indicate the normalized temperature increase throughout the body at various dimensionless times τ . The results indicate the finite element method gives accurate answers for this type problem.

Considering now the thermorheologically simple case where the dissipation function is dependent on temperature, it becomes impossible to nondimensionalize the problem under consideration in the same manner TAUCHERT [19] used for the isothermal problem; specific material properties must be employed. One common material used in many viscoelastic studies is Solithane[®] 113⁷, a polyurethane rubber whose characterization has been studied in detail by KNAUSS and

⁷ Trademark of Thiokol Chemical Corp., Trenton, New Jersey.

MUELLER [20]. Using a collocation technique, the tensile relaxation modulus data determined by KNAUSS and MUELLER was used to determine the constants in an exponential series expression. Assuming $G(t) = \frac{1}{3} E(t)$, the constants in the series expression for $G(t)$ in (30) were determined⁸ and are given in Table 1.

Table 1. *Relaxation Constants for Solithane*

i	τ_i (min)	G_i (psi)
1	1.0×10^{-12}	1653
2	1.0×10^{-11}	4747
3	1.0×10^{-10}	5539
4	1.0×10^{-9}	4701
5	1.0×10^{-8}	3527
6	1.0×10^{-7}	858
7	1.0×10^{-6}	257
8	∞	143

In a similar manner, an expression was obtained for the shift factor in the form of (32) with $K_1 = 0.60$, $K_2 = 8.89$, $K_3 = 183.5$ and $T_s = 89.6^\circ\text{F}$ and where the reference temperature for φ is 78°F .

Other pertinent properties of Solithane 113 employed in this study are:

coefficient of linear thermal expansion,	$\alpha = 1.46 \times 10^{-4}/^\circ\text{F}$,
conductivity,	$k = 8.56 \times 10^{-3}$ BTU/in-hr- $^\circ\text{F}$,
specific heat,	$c = 0.48$ BTU/lbm- $^\circ\text{F}$,
and density,	$\rho = 0.0361$ lbm/in ³ .

Consider now the same geometry as before, but for the case of thermorheologically simple material properties. Using the finite element method and the properties of Solithane 113, solutions were obtained to this problem for a frequency of 1000 cpm and a maximum strain γ_{0z} of 5%. The solution is illustrated in Fig. 3 along with the isothermal property solution. Including temperature dependent material properties is seen to produce a lower temperature rise in the sample than if isothermal properties are included.

5. Discussion and Conclusions

It has been demonstrated that Coleman's approach can be utilized to develop a consistent constitutive theory for thermorheologically simple materials. The results of this development agree conceptually with the corresponding equations developed using a phenomenological model approach.

It should be noted in deriving expressions for the stress, entropy, and dissipation function for thermorheologically simple materials using Coleman's

⁸ Knauss's data was shifted to a reference temperature of 78°F .

approach that the spatial gradient of the temperature was assumed small. This allows all points in the region of interest to be considered at the same value of reduced time which permits the balance principles to be applicable in reduced time. If the spatial gradient of the temperature is large, then the reduced time

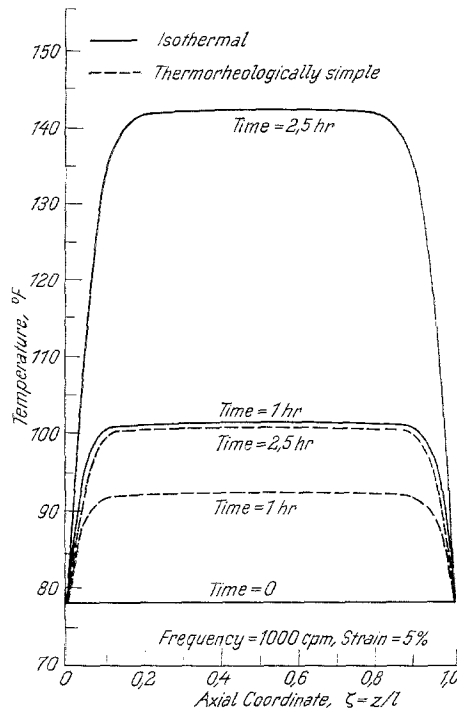


Fig. 3. Influence of temperature dependent properties on dissipation

varies from point to point within the region. This seems to prohibit application of the balance principles in terms of reduced time. The spatial derivative of the temperature complicates the form of the energy equation since the spatial derivative becomes

$$\left(\frac{\partial \theta}{\partial x}\right)_t = \left(\frac{\partial \theta}{\partial x}\right)_\xi + \left(\frac{\partial \theta}{\partial \xi}\right)_x \left(\frac{\partial \xi}{\partial x}\right)_t \quad (38)$$

in the reduced time variable.

The influence of thermorheologically simple material behavior on the heat generation phenomenon has been shown to be significant. Furthermore, improved computational methods are needed to calculate the dissipation function for noncyclic loads.

The utility of the finite element for solving thermomechanically coupled problems in complex geometries is apparent from the ease and accuracy with which the problem of the oscillating rod described here was solved.

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