Prediction of Temperature Gradients in Solid Propellants

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By employing uniaxial viscoelastic propellant data, it is demonstrated that normally neglected thermal gradients in propellant can affect the results of a stress analysis. It is shown that the stress analysis is significantly affected by discrepancies as small as 4°F from the true value, particularly for lower temperature states. Furthermore, it is shown that longitudinal temperature variations in a small operational motor can easily be 3°F, necessitating the employment of a three-dimensional thermal analysis as input to any viscoelastic stress analysis. Various analytical solutions predicting temperature distributions for a given problem are shown to have relative discrepancies of less than 2°F. A comparison of such analytical results, based on the use of reasonable constant thermal properties with results from an Air Force experiment in which reasonable experimental techniques were used, demonstrates that the prediction of temperature gradients are significantly affected by the temperature dependence of the thermal conductivity. Therefore, solutions obtained from the classical Fourier heat conduction equation, which becomes nonlinear if conductivity is not constant, can at best only be approximate.

Introduction

A COMPLETE viscoelastic characterization of a solid-propellant rocket grain necessitates the simultaneous prediction of stress, strain, temperature, and heat flow in the region of any point within the grain as functions of time. The traditional approach has been to predict the stress and strain response, given a particular thermal distribution. The contemporary method for elastic materials[1] and two typical methods for viscoelastic materials[2,3] still consider temperature and heat flow as known quantities and neglect coupling phenomena.[2] Several significant studies[4–7] have presented generally favorable comparisons between heat-transfer theory and experimental results after an iterative procedure was employed to obtain the proper material thermal properties. This after-the-fact technique is of limited value in the preliminary design of motors.

A closed-form solution to the transient thermal response of a finite-length, thick-walled cylinder does not exist because of the complexity associative with obtaining the solutions to the Fourier conduction constitutive equation.[8–10] The literature gives various solution ramifications of one-dimensional theory,[11–16] including a proposed method[17] that essentially superimposes the transient infinite plate and cylinder solutions. Fortunately, numerical methods[18,19] that reduce the three-dimensional Fourier equation to engineering practice are available as computer programs.[20–22]

This paper considers 1) temperature sensitivity of mechanical properties, 2) propellant thermal properties, 3) thermal analysis sensitivity to thermal properties, 4) temperature gradients in a finite thick-walled propellant cylinder modeled to the Air Force structural test vehicle (STV) motor, and 5) comparison of temperature predictions with STV thermocouple data.

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Temperature Sensitivity of Mechanical Properties

Reference 23 reports significant differences between theory and experiment for propellant uniaxial tensile-temperature interactions and that these differences were still substantial when Solithane 113 (an unfilled elastomer) was used instead of propellant. Bills et al.[24] state that grain stresses must be known quite accurately if the predictions based on cumulative damage are to be meaningful; e.g., the time to failure will change as much as 23.7% for a 1°F change in the temperature when the test temperature is −100°F.[25] At 200°F, the change in failure time is still large, 5.4%/°F.

A simple way to verify the influences of temperature (T) sensitivity on mechanical behavior is to examine a typical $\log a_t$ vs T curve, where a_t is the viscoelastic time temperature shift factor. It is recalled that the $\log a_t$ vs T curve is obtained by shifting uniaxial tension data from a series of short time-span, isothermal tests.[26] The least sensitive $\log a_t$ vs T curve found in the literature for a propellant was that in Ref. 27. By simply perturbing the temperature by, say, 4°F on the abscissa, a new value for $\log a_t$ is found on the ordinate. In a straightforward manner the change in modulus is found for different values of reduced time. The change in the uniaxial stress magnitude is then computed, given a strain level.

The results of this perturbation analysis are shown by the dashed lines in Fig. 1 for three temperature regimes. A change of 4°F from the true temperature will cause errors of 4.5%, 8%, and 15% in uniaxial tension for temperatures of 160°, 0°, and −60°F, respectively. This error would be significantly greater for a typical operational propellant because of the uncertainties created by experimental data scatter and the assumption that solid propellants are linearly viscoelastic.

To demonstrate further the temperature sensitivity of uniaxial stress, a typical error analysis[28] can be applied to an empirically obtained constitutive equation for a solid propellant, LPC-617P.[29] The results thus obtained are shown as the solid lines in Fig. 1. An error of 4°F will cause errors of about 5%, 8%, and 10% in uniaxial tension for temperatures of 160°, 0°, and −60°F, respectively. Although the uniaxial constitutive equation is only a first-order approximation based on curve-fitted uniaxial tension data, the predicted

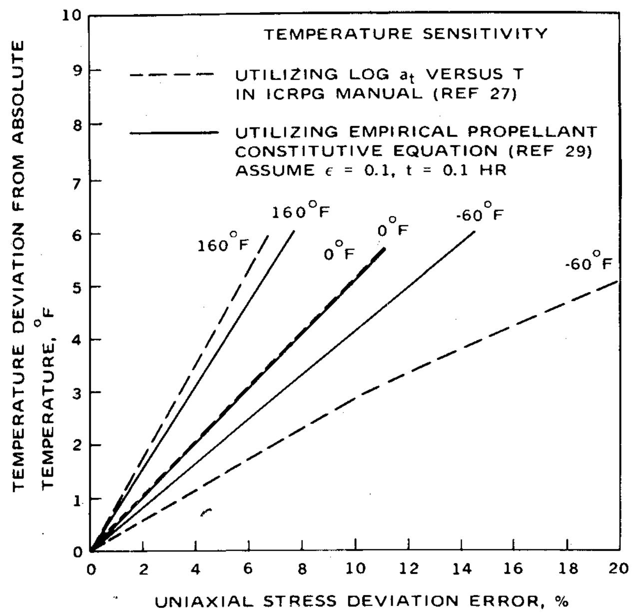


Fig. 1 Sensitivity of uniaxial stress to temperature uncertainties.

uniaxial stress deviation is close to that predicted by the log a_t vs T approach. Therefore, this second approach appears to confirm that a discrepancy of $\pm 4°F$ from the true temperature will introduce a significant error into a stress analysis.

Let us examine the approximate constitutive equation

$$\sigma = 8.16e^{2920/T}\,\epsilon^{0.484+0.00164T}t^{-0.436+7\times10^{-4}T} \tag{1}$$

Partial differentiation yields the sensitivity relations

$$\partial\sigma/\partial T = \sigma(0.0007 \ln t + 0.00164 \ln\epsilon^{-2920/T^2}) \tag{2}$$

$$\partial\sigma/\partial\epsilon = (3.95 + 0.01338T)e^{2920/T} \times t^{-0.436+7\times10^{-4}T}\epsilon^{-0.516+0.00164T} \tag{3}$$

$$\partial\sigma/\partial t = \sigma/t(-0.436 + 0.0007T) \tag{4}$$

where σ = uniaxial tension stress, psi; T = temperature, °R; t = time, hr; and ϵ = strain, in./in.

Typical results are shown in Table 1, which reveals that for a 4°F error in T, and no error in ϵ or t, the deviations in σ are the aforementioned value, i.e., 5%, 8%, and 10%. If the true ϵ is increased from 10% to 30%, the stress deviations become 4.5%, 7.1%, and 9%. Therefore, the strain level does not have a significant influence.

If T and t are precisely determined (i.e., $\Delta T = 0$, $\Delta t = 0$), and a discrepancy of 2% is experienced in the strain measurement, the deviations in σ are 30%, 25%, and 23% at a strain level of 10% and t = 6 min for T = 160°, 0°, and −60°F, respectively. At a strain level of 30%, the corresponding deviations in σ are 9.9%, 8.2%, and 7.5%. Thus, a 2% error in ϵ has the same magnitude of influence on computed σ as does a 4°F error in T, at typical ϵ levels encountered by operational motors.

If T and ϵ are precisely measured, and a discrepancy of 1% is experienced in t, the deviations in σ are 0, 1%, and 2% at ϵ = 0.1 and t = 6 min for T = 160°, 0°, and −60°F, respectively. At ϵ = 0.3, the corresponding deviations in σ are 0, 1.1%, and 1.6%. Thus, modest time errors do not appreciably affect the magnitude of computed σ.

Equation (1) is an empirical equation that approximately fits the uniaxial data for one propellant formulation. Although its value for sensitivity analysis has not been established, it may be useful to the preliminary design engineer.

Propellant Thermal Properties

Data on propellant thermal properties as functions of temperature are not readily available in the literature. Two sources[30,31] state that the thermal conductivity k can be measured within 4% and 5%, respectively. It is not clear whether these errors relate to accuracy or precision. Reference 32 states that it is difficult to obtain thermal measurements (for materials in general) more accurate than ±5% because of the many uncertainties encountered when using any of the steady-state or dynamic thermal measurement techniques.

The limited data available leave many questions to be answered. For example, for a polyurethane propellant TP-H-3062 (Surveyor), $k \simeq 0.19$ Btu/ft-hr-°F, increasing with temperature[33]; for a carboxy terminated polybutadiene (CTPB) propellant, $k \simeq 0.24$ Btu/ft-hr-°F and decreases with temperature[30]; for an unknown propellant, $k \simeq 0.15$ Btu/ft-hr-°F.[30] This variance for similar propellants is also exhibited by materials in general (Ref. 34, Tables 1.1 and 1.7). Therefore, it is suggested that the thermal property data available for thermo-mechanical analysis are subject to errors of at least ±5%.

An important parameter in thermal analysis is the coefficient of convective heat transfer h,[17,35] that either must be estimated or determined by an extremely well instrumented experiment. For engineering purposes, h can be back-calculated from modest experimental data. The range in values in Btu/ft²-hr-°F for free convection in gases range from 0.6 to 4 and in water from 20 to 125. For forced convection, h ranges from 10 to 100 in gases and from 100 to 2000 in water. It is obvious that significant errors can be made by not knowing a reasonable value for h.

Thermal Analysis Sensitivity to Thermal Properties

The sensitivity of predicted temperature gradients and heat flow with variable k at a point in the interior of a propellant grain can be readily demonstrated for an infinitely long cylinder with two isothermal surfaces.[16] In Ref. 33, dk/dT for TP-H-3062 propellant is 0.0007 Btu/ft-hr-°F/°F. If a thick-walled cylinder has a 7.0 in. o.d. and a 2.6 in. i.d., and the isothermal temperature on the outside and

Table 1 Uniaxial stress deviation $\Delta\sigma$ due to small perturbations in temperature, strain, and time at t = 0.1 hr

ϵ → %	T, °R	σ, psi	ΔT, °R	$\Delta\epsilon$, %	Δt, hr	$\Delta\sigma$ → %
10	614	31.1	4	0	0	5.1
			0	2	0	30
			0	0	0.01	0
	454	393	4	0	0	7.9
			0	2	0	25
			0	0	0.01	1
	394	1446	4	0	0	9.7
			0	2	0	23
			0	0	0.01	2
30	614	160	4	0	0	4.5
			0	2	0	9.9
			0	0	0.01	0
	454	1516	4	0	0	7.1
			0	2	0	8.2
			0	0	0.01	1.1
	394	5007	4	0	0	9.0
			0	2	0	7.5
			0	0	0.01	1.6

inside surfaces are 90° and 0°F, the temperature in the radial center will deviate 0.7°F, and the heat flow at this point will deviate 3% from the solution based on constant k. If there is a significant discrepancy in k such as is indicated between Refs. 30 and 33 (possibly ±0.05 Btu/ft-hr-°F), an error of ±15°F in temperature is possible.

Temperature Gradients in a Finite Thick-Walled Cylinder

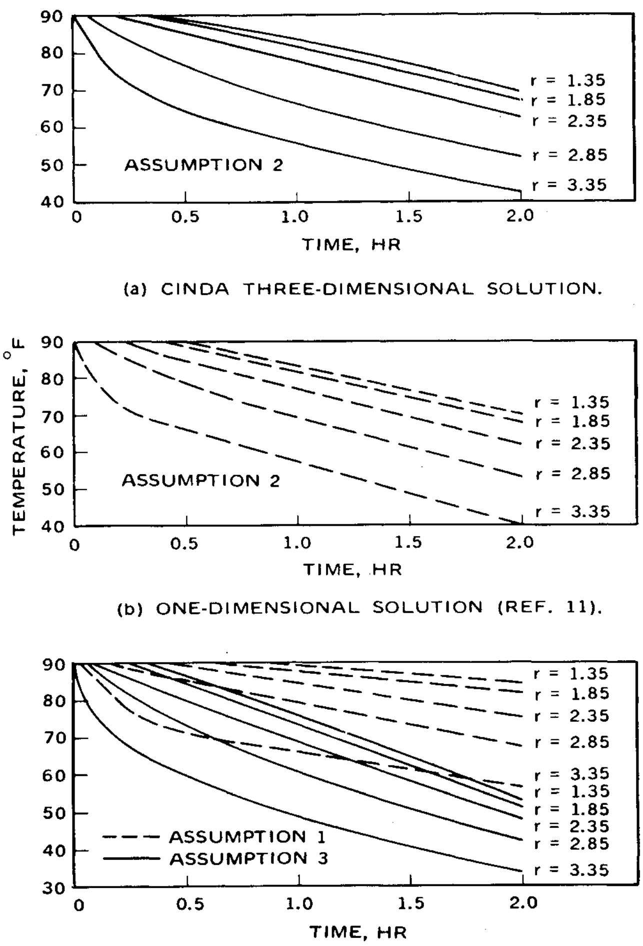
Because modest temperature errors do introduce significant errors in σ at low temperatures, two questions of interest are as follows. Must a three-dimensional (3D) thermal analysis be used in thermomechanical stress analysis because of appreciable longitudinal temperature gradients? Are there significant differences in temperature gradients peculiar to the particular analytical technique employed? The answers to these questions are found by utilizing the finite-difference[20] and finite-element[21,22] transient thermal programs.

The mathematical model to be examined is analogous to the Air Force STV motor.[36,37] The model grain is 7-in. o.d. × 2.62 in. i.d. × 35 in. long. The thermal properties, assumed to be independent of temperature (since appropriate data were not available) are k = 0.2 Btu/ft-hr-°F, specific heat, (c_p) = 0.3 Btu/lb-°F, density, (ρ) = 113 lb/ft^3 (hence diffusivity, $\alpha = k/c_p\rho$ = 0.00584 ft^2/hr); and h = 1.2 Btu/ft^2-hr-°F. The accuracy of these values is relevant only if a direct comparison is to be made with a particular experiment, but they are reasonable approximations for preliminary design. The initial temperature is 90°F, and the grain is subjected to an air temperature of 0°F. Convective heat transfer is assumed for the entire outer boundary. The port is insulated, i.e., the port volume is thermally sealed and the resulting air pocket is assumed to have negligible conductivity. The effects of thermal resistance and capacitance of the container are neglected here, but they can be incorporated in the analysis for on infinite cylinder.[38] The mathematical grid incorporated a symmetrical plane quarter of the grain and consisted of 350 nodes for the (Chrysler Improved Numerical Differencing Analyser) program,[20] 396 nodes for the Rohm and Haas (R&H) program[21] and 98 nodes for the University of California (UC) program.[22] The results for three longitudinal stations (z's) for these three programs are given in Table 2 for the time of 1 hr.

The CINDA and R&H programs predict a temperature drop between z = 17.5 and z = 2 of ~3°F. The differences between the two programs range from ~1° to ~6°F. The UC program matches the boundary nodes of CINDA and R&H, but predicts smaller longitudinal temperature drops (<1°F). Obviously better agreement would be found if the full potential of each program were utilized. However, it would be unreasonable to assume that the full potential of each program would be employed during the preliminary design phase because thermal properties for proposed new propellant formulations are usually only estimated to begin with.

Table 2 Longitudinal temperature predictions using three different computer programs

		T,°F		
z, in.	r, in.	CINDA	R&H	UC
0	3.35	42.2	37.9	37.3
	2.35	54.5	50.0	52.5
	1.35	58.1	54.0	57.2
≈2	3.35	52.3	58.0	54.3
	2.35	74.2	74.7	76.2
	1.35	80.1	82.3	83.0
17.5	3.35	55.6	59.6	54.8
	2.35	77.6	76.8	77.0
	1.35	83.9	84.6	83.9



(a) CINDA THREE-DIMENSIONAL SOLUTION.

(b) ONE-DIMENSIONAL SOLUTION (REF. 11).

(c) EXTREME VARIATIONS DUE TO THERMAL PROPERTIES.

Fig. 2 Temperature gradients at longitudinal center line for various radial locations. See Table 4 for assumptions 1–3.

The transient temperature response (to 2 hr) is shown in Fig. 2a for CINDA for five selected radial nodes at z = 17.5 (centerline). The results for R&H and UC are similar, noting the typical discrepancies among the three programs in Table 2. A reasonable comparison of CINDA results and those obtained by superimposing the infinite cylinder with infinite plate transient thermal solutions[17] gives a discrepancy of ~3°F at 1.8 hr. However, for shorter times, the latter technique breaks down completely.

Table 3 compares results from the UC program for the three-dimensional and one-dimensional analyses at the longitudinal center line. The latter, for a finite cylinder, is obtained by employing the technique of Ref. 11 as shown in Fig. 2b. A comparison of Figs. 2a and 2b shows good agreement up to 2 hr (deviations of up to 2°F). The discrepancy between these solutions is modest, with the three-dimensional solution predicting a lower temperature (≈1°F). Such discrepancies may be caused by errors in numerical technique, for it is unreasonable to expect that the results reported should be identical. The important point is that the computational error can be easily of the order of ±2°F.

Let us now examine the sensitivity of the analysis to thermal property perturbations. A set of reasonable thermal data for the STV motor (CTPB) was used to obtain the results of Fig. 2a. Specific heat is said to be measured within 10%, k within 50%, and h can be estimated within 100%. Thermal data assumptions 1 and 3 of Table 4 can be used to determine the two extremes of predicted temperature range.

For the one-dimensional analysis, the transient temperature gradients using the data in Table 4 are shown in Figs. 2b and 2c. Figure 2c also shows the extreme temperature limits based on assumptions 1 and 3. The thermal property values used in the three-dimensional analysis are those of assumption 2 and are shown in Fig. 2a, which compares very favorably (2°F) with the one-dimensional analysis shown in Fig. 2b. By referring to Fig. 2c it is seen that deviations of 15°F from the values of Fig. 2b can exist at the longer times. Therefore, both analytical solutions are fairly sensitive to modest changes in physical properties. In rough terms, changes that enhance k cause the curves to rotate clockwise; changes in h slightly change the gap width between radial points 1 and 5. Hence, it is possible to backfit theoretical predictions to satisfy any one set of experimental data.

Comparison of Theory with Experiment

Pertinent thermal transient data[36] for a long, thick-walled, cylindrical CTPB propellant motor were obtained from five radially spaced embedded thermocouples (Fig. 3a) at the longitudinal center of the motor. The propellant grain was entirely encased in a 0.375-in.-thick steel case, whose temperature was also monitored with a thermocouple. The initial equilibrium motor temperature was 90°F. The reported experiment consisted of obtaining transient temperature measurements at various radial points as the motor was cold-soaked at approximately 0°F in an air chamber (Fig. 3b). It is seen that the thermocouple experienced cycling of a few degrees from the assumed mean temperature; no error analysis of the experiment nor accurate thermal properties were available.

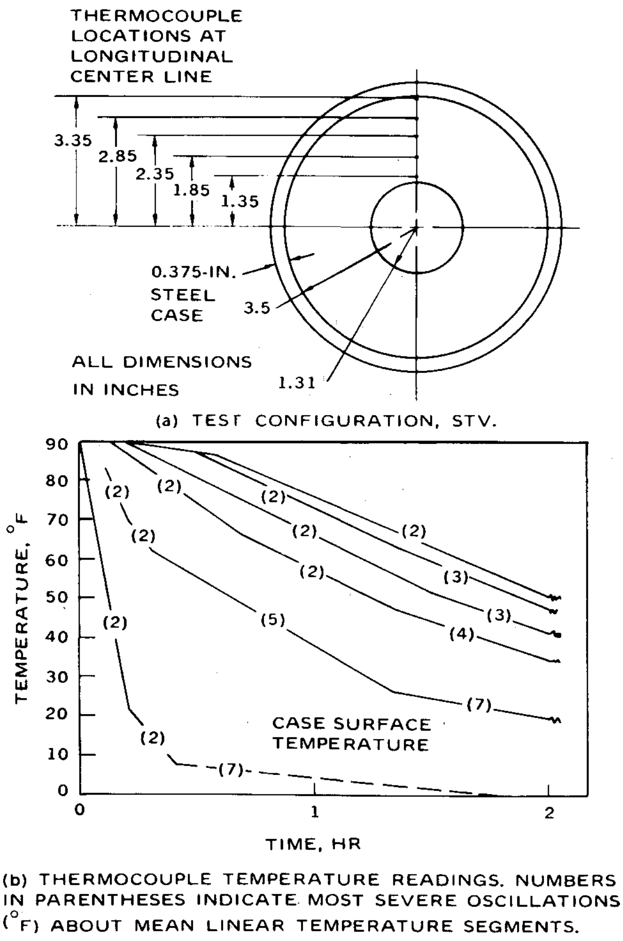


Fig. 3 Thermocouple readings for one STV CTPB motor at longitudinal center line.

Table 3 Three-dimensional (3D) vs one-dimensional (1D) temperature distribution at center line

r, in.	Geometry	T, °F 0.2 hr	0.6 hr	1 hr	1.8 hr
1.97	3D	89.4	85.9	80.8	69.2
	1D	88.4	86.3	81.4	70.5
2.41	3D	88.6	83.2	77.0	65.6
	1D	88.6	83.2	77.0	65.6
2.85	3D	86.9	78.8	71.5	60.0
	1D	86.4	77.6	70.1	58.7
3.06	3D	83.2	71.9	64.1	53.1
	1D	84.1	73.4	65.7	54.6

A comparison of Fig. 3b with Fig. 2, that employed reasonable values for c_p, h, k, and ρ indicates a significant discrepancy. Since various analytical methods were employed and each gave the same solution to the Fourier heat conduction equation (thus validating the given solution), one would suspect serious error either in the constant thermal property values used or in the method of obtaining the experimental data, or both. Further light may be shed on this serious discrepancy if the experimental temperature thermocouple data are assumed to be relatively correct. Then such data may be used to investigate from a different point of view the Fourier heat conduction equation, which is the basis for the theoretical solutions given in Fig. 2.

The Fourier heat conduction equation, in cylindrical coordinates, assuming only radial heat flow, is

$$\partial T/\partial t = \alpha[\partial^2 T/\partial r^2 + (1/r)\partial T/\partial r] \tag{5}$$

where $\alpha = k/\rho c_p$ is the thermal diffusivity. It is noted that possible energy transfer mechanisms such as strain energy are not explicitly included in the energy balance. Hence, only three physical properties are assigned to characterize temperature gradients.

To use Fourier's equation in the form shown in Eq. (5), one assumes the following: only one-dimensional heat flow occurs, k is a constant over the temperature range considered, the material must be homogeneous and isotropic, there are no internal heat sinks or sources, the material is a perfect continuum, the vectors of heat flux and of the temperature gradients are collinear, and heat flux is directly proportional to the magnitude of only the temperature gradient. The degrees of validity of these assumptions with respect to thermal gradients in a filled composite propellant have not been established. Analogous assumptions are made in classical elasticity theory that, when applied to solid propellants, have been shown not to be applicable (e.g., composite propellants dewet with strain).

The value of α used to obtain the results in Fig. 2b was 0.00584 ft²/hr. The solutions in Fig. 2 required that α be constant over the temperature range considered. This requirement can be examined by calculating α from Eq. (5), after graphically differentiating the experimental temperature data of Fig. 3 at each thermocouple location at times of 1 hr and 2 hr; the results in Fig. 4; show that α is not a constant. Thus, classical one-dimensional solutions using the Bessel function approach cannot be expected to give

Table 4 Spectrum of reasonable values of k and h for the STV motor; c_p = 0.3 Btu/lb-°F; ρ = 113 lb/ft³

Assumption	k, Btu/ft-hr-°F	h (air chamber), Btu/ft²-hr-°F
1	0.1	0.6
2	0.2	1.2
3	0.3	2.0

Table 5 Effective and average temperature at three times

	0.5 hr	1 hr	2 hr
T_{centroid}, °F	84	69	44
h, Btu/ft²-hr-°F	0.3	1.2	3.0

accurate theoretical solutions to the Fourier equation, since α is temperature-dependent. Moreover, α must be a function of other variable(s), since the slopes in Fig. 4 change with time. There also appears to be an accelerating lowering of α for lower temperatures. The temperature dependence of α can be further assessed by assuming the k, c_p, and ρ are the only variables to affect α. If k and ρ are assumed constant, then it is possible to separate the c_p contribution by employing

$$c_p = 0.3 - 0.00271\Delta T \tag{6}$$

that was obtained from Ref. 33. The effect of α of such a $c_p(T)$ is shown as the dashed lines in Fig. 4, which are essentially vertically displaced from the solid curves. Therefore, the basic temperature dependence of α appears to be primarily a function of k. The rotation effect may be largely attributed to changes in c_p.

The values for k can be computed for α using the assumed values of c_p and ρ. These values are shown in Fig. 4 (with the ordinate on the right side) as a solid curve for a constant c_p (0.3 Btu/lb-°F) and as a dashed curve for a temperature-dependent c_p [Eq. (6)]. Now it appears that k is a strong function of temperature (and other variables). Note that the value of k used in the numerical analysis was 0.2 Btu/ft-hr-°F and was considered as a reasonable representative average such as would be obtained from a guarded hot plate apparatus (steady-state equilibrium measurement).

It should be noted too, that there are no commonly accepted data for $k = k(T)$ in the literature for solid propellants. Some very approximate data are given in Refs. 30 and 33. One reason for this is the difficulty associated with designing appropriate apparatus.[39] Hence, k data tend to be quite subjective; furthermore the reproducibility of the data by the various laboratories[39,40] is poor. One would not expect to find a good correlation between k values obtained from a guarded hot plate apparatus (one-dimensional heat flow) and from the motor soak test (two-dimensional heat flow); however, the temperature gradients are severely influenced by modest changes in k.

The value for h used in the analysis was 1.2 Btu/ft²-hr-°F, obtained by assuming free convection of air on a cylinder (Ref. 41), and compares favorably with that used elsewhere (h = 1.8 Btu/ft²-hr-°F for a 5-in. o.d. grain in Ref. 24, p. 23). The validity of this value can also be estimated from the experimental data (Fig. 3) in the following way.

Assume that the average thermal properties of the propellant grain are those located at its mass centroid $\bar{r}$. The temperature at this radial position is obtained by interpolation from Fig. 3. The lumped-heat-capacity method[17] is then employed. Instead of using the general interpretation of h (flow convection coefficient), an analogous h (contact conductance) is computed using the empirical Newtonian cooling hypothesis. The h then computed does not have the interpretation associated with boundary-layer theory. However, the boundary heat-transfer mechanism need not be known for this problem. The heat-transfer model assumed is that of a propellant point mass (no thermal gradients) connected to the steel environment according to the Newtonian heat hypothesis, where h is interpreted as the quantity necessary to transfer the heat flux from the single point mass to the environment. The relationship of h, so defined, to the mass centroid temperature is given by

$$T_{\text{ntioid}} - T_{\text{steel}}/T_{\text{initial}} - T_{\text{steel}} = e^{-(hA/\rho c_p V)t} \tag{7}$$

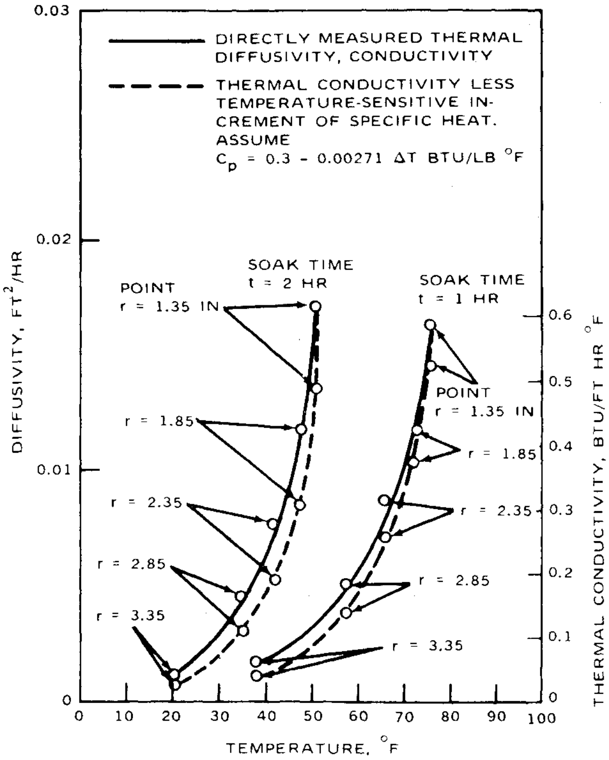


Fig. 4 Experimental thermal diffusivity and consequential thermal conductivity as a function of temperature.

where A is the area (ft²) through which the heat flows, and V is the volume (ft³) of the propellant mass. In Table 5 are the computed values of h for $\bar{r}$ = 2.6 in., c_p = 0.3 Btu/lb-°F, and ρ = 113 lb/ft³ at various times. Accordingly, the value for h employed for the boundary conditions in the theory was reasonable.

Summary and Conclusions

It appears that viscoelastic stress analysis is significantly affected by discrepancies of only 4°F from the true value, especially at low temperatures (<0°F). Since longitudinal temperature variations of 3°F can easily occur in grains, a three-dimensional thermal analysis is therefore essential for propellant stress analysis. Errors ≤2°F are intrinsic to the various analytical methods. A comparison of analytical results incorporating reasonable thermal properties with a well controlled Air Force experiment demonstrated that the prediction of temperature gradients is significantly affected by the temperature dependence of the thermal conductivity. Modest longitudinal temperature gradients, currently ignored in thermal and viscoelastic stress analyses, should be considered.

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