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FREQUENCY DEPENDENT THERMAL EXPANSION OF VISCOELASTIC COMPOSITES

James G. Berryman
Geophysics Department
Earth Sciences Division
Lawrence Berkeley National Laboratory
Berkeley, CA

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QUICK REVIEW OF SOME NOTATION

Common Averages of Quantity Q

- MEAN:

$$Q_{mean} = \langle Q \rangle = \sum f_i Q_i$$

- HARMONIC MEAN:

$$Q_{harm} = \left\langle \frac{1}{Q} \right\rangle^{-1} = \left[\sum \frac{f_i}{Q_i} \right]^{-1}$$

- GEOMETRIC MEAN:

$$log\, Q_{geo} = \langle log\, Q \rangle = \sum f_i\, log\, Q_i \quad \text{OR}$$

$$Q_{geo} = \Pi_i Q_i^{f_i}$$

Note: $\sum_i f_i = 1$ (for our applications f_i is typically the volume fraction of the i-th constituent).

Canonical Functions (Real or Complex)

- **For electrical conductivity σ:**

$$\Sigma(s) = \left\langle \frac{1}{\sigma(\vec{r}) + 2s} \right\rangle^{-1} - 2s$$

- **For bulk modulus K:**

$$\Lambda(u) = \left\langle \frac{1}{K(\vec{r}) + \frac{4}{3}u} \right\rangle^{-1} - \frac{4}{3}u$$

- **For shear modulus G:**

$$\Gamma(z) = \left\langle \frac{1}{G(\vec{r}) + z} \right\rangle^{-1} - z$$

Extreme Limits of the Canonical Functions Whether Real or Complex

When arguments are as low or high as possible (0 or ∞), the results for all these canonical functions produce the mean or the harmonic mean of the physical quantity involved.

For example, the bulk modulus K-related function gives:

$$\Lambda(0) = \left\langle \frac{1}{K(\vec{r})} \right\rangle^{-1}$$

$$\Lambda(\infty) = \langle K(\vec{r}) \rangle$$

These facts are important for motivating the use of Milton's closely related Y-transform.

General Inequalities (for Real Quantities Q)

- **For electrical conductivity σ:**

$$0 \le \sigma_{min} \le \left\langle \sigma(\vec{r})^{-1} \right\rangle^{-1} \le \sigma_{eff} \le \langle \sigma(\vec{r}) \rangle \le \sigma_{max} \le \infty$$

- **For bulk modulus K:**

$$0 \le K_{min} \le \left\langle K(\vec{r})^{-1} \right\rangle^{-1} \le K_{eff} \le \langle K(\vec{r}) \rangle \le K_{max} \le \infty$$

- **For shear modulus G:**

$$0 \le G_{min} \le \left\langle G(\vec{r})^{-1} \right\rangle^{-1} \le G_{eff} \le \langle G(\vec{r}) \rangle \le G_{max} \le \infty$$

Hashin-Shtrikman Bounds for Real Q's (1)

- **For electrical conductivity σ:**

$$\sigma_{HS}^{-} \leq \sigma_{eff} \leq \sigma_{HS}^{+},$$

where

$$\sigma_{HS}^{-} = \Sigma(\sigma_{min}) \text{ and } \sigma_{HS}^{+} = \Sigma(\sigma_{max})$$

- **For bulk modulus K:**

$$K_{HS}^{-} \leq K_{eff} \leq K_{HS}^{+},$$

where

$$K_{HS}^{-} = \Lambda(G_{min}) \text{ and } K_{HS}^{+} = \Lambda(G_{max})$$

Hashin-Shtrikman-Walpole Bounds for Real G's (2)

- **For shear modulus G:**

$$G_{HS}^{-} \leq G_{eff} \leq G_{HS}^{+},$$

where

$$G_{HS}^{-} = \Gamma(\zeta_{min}) \text{ and } G_{HS}^{+} = \Gamma(\zeta_{max})$$

with

$$\zeta_{min} = \tfrac{G_{min}}{6}\tfrac{9K_{min}+8G_{min}}{K_{min}+2G_{min}}$$
$$\zeta_{max} = \tfrac{G_{max}}{6}\tfrac{9K_{max}+8G_{max}}{K_{max}+2G_{max}}.$$

HS only considered well-ordered case $(K_1 - K_2)(G_1 - G_2) > 0$.

Walpole considered general case, so these are called HSW bounds.

Self-Consistent (SC) Method or Coherent Potential Approximation (CPA) for Isotropic Composites

- **For electrical conductivity σ:**

$$\sigma^* = \Sigma(\sigma^*)$$

- **For elastic constants (bulk K and shear G):**

$$K^* = \Lambda(G^*)$$
$$G^* = \Gamma(\zeta^*),$$

where

$\zeta^* = (G^*/6)(9K^* + 8G^*)/(K^* + 2G^*)$ depends on both K^* and G^*.

OUTLINE

- Quick Review of Some Notation
- Two-Component Thermoviscoelastic Composites
    - Thermal expansion: exact results
    - Some theoretical development for bulk viscoelasticity
    - Frequency dependence
- Bounds on Complex Elastic Moduli
    - Bulk modulus
    - Complex thermal expansion
- Discussion and Conclusions

Two-Component Thermoviscoelastic Composites

The general equation of interest is:

$$\begin{pmatrix} \delta e \\ -\delta s \end{pmatrix} = \begin{pmatrix} \frac{1}{K} & 3\beta \\ 3\beta & c_p \end{pmatrix} \begin{pmatrix} -\delta p_c \\ -\delta\theta \end{pmatrix},$$

where δe is the strain increment, δs is the entropy increment, δp_c is the confining pressure increment, and $\delta\theta$ is the temperature increment. K is the bulk modulus, β is the thermal expansion coefficient, and c_p is the heat capacity.

Using subscripts 1 and 2 will identify the coefficients and fields as belonging to constituents 1 and 2. Using superscript $*$ will identify the corresponding overall effective property.

Thermal Expansion: Exact Results (1)

Consider a thought experiment wherein we ask the question whether it might be possible to find some combination of the uniform fields $\delta p_c^* = \delta p_1 = \delta p_2$ and $\delta\theta^* = \delta\theta_1 = \delta\theta_2$ such that the strains in the two components are equal $\delta e_1 = \delta e_2$ and therefore also equal to the overall strain δe^*.

This set of conditions holds if (and only if)

$$\delta e^* = -\tfrac{\delta p_1}{K_1} - 3\beta_1\delta\theta_1$$

$$= -\tfrac{\delta p_2}{K_2} - 3\beta_2\delta\theta_2 = -\tfrac{\delta p^*}{K^*} - 3\beta^*\delta\theta^*.$$

Thermal Expansion: Exact Results (2)

These conditions imply specifically that the special value of the ratio $\frac{p_c}{3\theta}$ for which this condition must hold is:

$$\frac{p_c}{3\theta} = \frac{\beta_2 - \beta_1}{\frac{1}{K_1} - \frac{1}{K_2}}.$$

As long as this condition is not disallowed by a special choice of the parameters (such as $K_1 = K_2$), then the thought experiment is successful and we have an exact result for β^*.

Thermal Expansion: Exact Results (3)

The results are:

$$\beta^* = \langle\beta\rangle + \frac{p_c}{3\theta}\left[\left\langle\frac{1}{K}\right\rangle - \frac{1}{K^*}\right]$$

where, for the special circumstances under consideration, we have:

$$\frac{p_c}{3\theta} = \frac{\beta_2 - \beta_1}{\frac{1}{K_1} - \frac{1}{K_2}}.$$

Combining these two results gives the final formula we need:

$$\beta^* = \langle\beta\rangle + \frac{\beta_2 - \beta_1}{\frac{1}{K_2} - \frac{1}{K_1}}\left[\frac{1}{K^*} - \left\langle\frac{1}{K}\right\rangle\right]$$

This result is formally identical to the corresponding results of Cribb (1968), Rosen and Hashin (1970), and many others.

The important difference is that this result is valid for the case of complex bulk moduli K_1, K_2. It shows that β^* itself is generally complex in composite viscoelastic media.

Some Theoretical Development (1)

Defining complex strain ϵ, complex stress σ,
and complex stiffness C (which varies in space because of the presence of two distinct constituents), we have the viscoelastic constitutive relationship:

$$\sigma = C\varepsilon.$$

Think of this as a 6 × 6 system of equations:
σ and ε are each 1×6 complex vectors, and
C is a 6×6 complex matrix (using the Voigt convention for transforming elastic or viscoelastic tensors to matrices).

Some Theoretical Development (2)

If real parts are distinguished by single primes and imaginary parts by double primes, then we can define real, composite vectors

$$j = \begin{pmatrix} \varepsilon'' \\ \sigma'' \end{pmatrix} \quad \text{and} \quad e = \begin{pmatrix} -\sigma' \\ \varepsilon' \end{pmatrix},$$

and a corresponding 12 × 12 system

$$j = De,$$

where now

$$D = \begin{pmatrix} (C'')^{-1} & (C'')^{-1}C' \\ C'(C'')^{-1} & C'' + C'(C'')^{-1}C' \end{pmatrix}$$

is a 12 × 12 real matrix.

Some Theoretical Development (3)

So, there is still a lot of work to do, but now we are dealing just with real quantities. We have to analyze the behavior of the average D matrix for our binary composite, but this is relatively straightforward now within the context of the random media theory. We can just generalize the Hashin-Shtrikman variational principle for this more general problem. This results in bounds on both complex bulk modulus and complex shear modulus.

We are going to skip over these details here, so I can show you some related developments concerning the canonical functions and the so-called Y-tensor.

Complex Bulk Modulus Bounds (1)

Define four points in the complex plane, using the complex version of the canonical functions, *i.e.*, same definition of the function but the bulk moduli appearing in the expression and also the arguments are considered complex (but f_1, f_2 always real):

$$K_{1*} = \Lambda(G_1)$$

$$K_{2*} = \Lambda(G_2)$$

$$K_{h*} = \Lambda(0) = \left\langle \frac{1}{K(\vec{r})} \right\rangle^{-1}$$

$$K_{a*} = \Lambda(\infty) = \langle K(\vec{r}) \rangle = f_1 K_1 + f_2 K_2.$$

The values of K_1 and K_2 are now those of the complex bulk moduli of the two viscoelastic constituents.

Complex Bulk Modulus Bounds (2)

Gibiansky and Milton define four arcs in the complex K-plane, each arc passing through the first two points ($p = K_{1*}$,K_{2*}), and also through one of the remaining four points (p) according to:

$$\mathrm{Arc}(K_{1*}, K_{2*}, K_{h*}), \quad \mathrm{Arc}(K_{1*}, K_{2*}, K_{a*}),$$
$$\mathrm{Arc}(K_{1*}, K_{2*}, K_{1}), \quad \mathrm{Arc}(K_{1*}, K_{2*}, K_{2}),$$

where

$$\mathrm{Arc}(p_1, p_2, p_3) \equiv \gamma_1 p_1 + \gamma_2 p_2 - \frac{\gamma_1\gamma_2(p_1-p_2)^2}{\gamma_2 p_1+\gamma_1 p_2-p_3},$$

and $\gamma_1 = 1 - \gamma_2$ is real and varies along [0,1].

This is a linear fractional, or bilinear, transformation.

Canonical Functions and the Y-Tensor (1)

Let the actual effective constants be K^* and G^*.

Then, with the definitions given before of Λ and Γ,

we can define arguments Y_K^* and Y_G^* such that

$$K^* = \Lambda(3Y_K^*/4) \quad \text{and} \quad G^* = \Gamma(Y_G^*).$$

Since the canonical functions are one-to-one, they are invertible

for arguments in terms of other quantities:

$$Y_K^* = \frac{K_1K_2(K^*{<}1/K{>}-1)}{{<}K{>}-K^*},$$

$$Y_G^* = \frac{G_1G_2(G^*{<}1/G{>}-1)}{{<}G{>}-G^*}.$$

This fact is very useful because, if we can bound these Y's,

then we obtain rather tight bounds on K^* and G^*.

Canonical Functions and the Y-Tensor (2)

In the present context, we can define the general Y^*-tensor according to:

$$Y^*(D^*, D_1, D_2) = \begin{pmatrix} (y'')^{-1} & -(y'')^{-1}y' \\ -y'(y'')^{-1} & y'' + y'(y'')^{-1}y' \end{pmatrix},$$

where the complex 6×6 matrix y is defined by

$$y(C^*, C_1, C_2) =$$
$$-f_2C_1 - f_1C_2 + f_1f_2(C_1 - C_2)(f_1C_1 + f_2C_2 - C^*)^{-1}(C_1 - C_2).$$

This matrix can be broken down into its bulk and shear parts.

Canonical Functions and the Y-Tensor (3)
Shear Modulus Example

When this has been done for shear, we can show (. . .) that:

$$\begin{pmatrix} \frac{1}{2y''_G} & -\frac{y'_G}{y''_G} \\ -\frac{y'_G}{y''_G} & 2\left[y''_G + \frac{(y'_G)^2}{y''_G}\right] \end{pmatrix} - Z \geq 0.$$

Here Z is a 2×2 real comparison matrix. This statement says that the spectrum of the 2×2 matrix on the left must be nonnegative. So its eigenvalues must be nonnegative. After some more algebra, we can show that this implies the point $y'_G + iy''_G$ must lie inside definite circles in the complex Y_G-plane. The matrix Z contains some parameters that we are free to vary, and the final bounds lie inside the convex hull generated by considering all these bounding circles.

Complex Hashin-Shtrikman-Walpole Points

The complex shear modulus, just as in the case of real coefficients, depends on a combination of the bulk and shear moduli of the constituents. But, unlike the real case, there are four of these points that need not fall in any simple order on the complex plane. They are:

$$\begin{aligned}
Y_{11} &= y(K_1, G_1) = \tfrac{G_1}{6}\tfrac{9K_1+8G_1}{K_1+2G_1},\\
Y_{22} &= y(K_2, G_2) = \tfrac{G_2}{6}\tfrac{9K_2+8G_2}{K_2+2G_2},\\
Y_{12} &= y(K_1, G_2) = \tfrac{G_2}{6}\tfrac{9K_1+8G_2}{K_1+2G_2},\\
Y_{21} &= y(K_2, G_1) = \tfrac{G_1}{6}\tfrac{9K_2+8G_1}{K_2+2G_1}.
\end{aligned}$$

We call these the Hashin-Shtrikman-Walpole points, by analogy to the case of real coefficients. They turn out to be important points for the shear modulus bounds and estimates.

EXAMPLES:

Some numerical examples will be displayed separately.

DISCUSSION: SOME APPLICATIONS

○ Viscoelastic liquid-liquid mixture: complicated composite liquid viscosity effects, relatively simple thermal expansion

○ Viscoelastic liquid-solid mixture (suspension) dominated by the liquid: similar to the liquid-liquid mixture

○ Viscoelastic solid-liquid mixture (porous medium) dominated by the solid: similar to the solid-solid mixture

○ Viscoelastic solid-solid mixture: complicated composite solid viscoelastic and thermoelastic effects

CONCLUSIONS

- Thermal expansion in two-phase viscoelastic composites is frequency dependent, and bounds on the viscoelastic bulk modulus are required to obtain the pertinent bounds on the complex thermal expansion coefficient.

- The use of uniform coupled fields for two-component media is very helpful in this application as it shows how to obtain exact results relating the thermal expansion to the overall viscoelastic bulk modulus.

- The ideas have many applications from fluid-fluid to solid-solid composites, and all mixtures in between – including porous media.

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