Exact results in linear thermomechanics of fluid-saturated porous media

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Abstract

Exact results are derived relating the various bulk moduli (frame, unjacketed, and pore) and heat capacity of inhomogeneous fluid-saturated porous media to the pertinent thermal expansion coefficients and component moduli when only two porous solid constituents are present. The porous solids need not be space filling or in perfect welded contact, so these results apply to materials containing some voids or cracks interspersed between the two constituents in addition to the interior voids associated with their pores. The key ratio of fluid pressure to temperature change producing uniform expansion or contraction is shown to be independent of porosity.
Using arguments similar to those used by Cribb\textsuperscript{1} and Schulgasser\textsuperscript{2} for thermoelasticity, Berryman and Milton\textsuperscript{3} have recently shown that exact relations may be obtained for a porous material composed of only two porous constituents that completely fill the volume of the composite (except for the pore space within themselves). Although these results dramatically improve our modeling capability compared to that of Gassmann's equation\textsuperscript{4} (derived assuming only a single solid constituent is present), the assumption that the two porous components must be volume filling is very restrictive and precludes using this analysis for the common situation in rocks and other porous materials where other voids and cracks are present. It is the purpose of this paper to point out that, by introducing another field (temperature), we can obtain exact results for two constituents plus voids, thus eliminating this unpleasant restriction imposed by the previous approach. This idea is similar to Schulgasser's approach to analyzing three component polycrystalline composites.\textsuperscript{2}

For isotropic materials and hydrostatic pressure variations, the three independent variables in linear thermomechanics of porous media are the confining (external) pressure $p_c$, the fluid (pore) pressure $p_f$, and the temperature $\theta$. The differential pressure $p_d \equiv p_c - p_f$ is often used to eliminate the confining pressure. The equations of the fundamental dilatations are

\[
- \frac{\delta V}{V} = \frac{\delta p_d}{K} + \frac{\delta p_f}{K_s} - 3\alpha \delta \theta
\]

for the total volume $V$, \hfill (1)

\[
- \frac{\delta V_\phi}{V_\phi} = \frac{\delta p_d}{K_p} + \frac{\delta p_f}{K_\phi} - 3\alpha_\phi \delta \theta
\]

for the pore volume $V_\phi$, and \hfill (2)

\[
- \frac{\delta V_f}{V_f} = \frac{\delta p_f}{K_f} - 3\alpha_f \delta \theta
\]

for the fluid volume $V_f$. Equation (1) serves to define the various constants of the porous solid, such as the drained frame bulk modulus $K$, the unjacketed bulk modulus $K_s$, and the coefficient of linear thermal expansion $\alpha$ for the composite frame. Similarly, (3) defines the bulk modulus $K_f$ and linear thermal expansion coefficient $\alpha_f$ of the pore fluid. Although reciprocity\textsuperscript{5} shows that $K_p = \phi K/(1 - K/K_s)$ where $\phi$ is the porosity, the remaining bulk modulus $K_\phi$ in (2) is independent of the others and (with rare exceptions\textsuperscript{6}) has seldom been estimated and never been measured for composite porous materials such as rocks. The thermal expansion coefficient $\alpha_\phi$ for the pore space has been introduced previously by McTigue\textsuperscript{7}, but no measured values of this coefficient are available.

Treating $\delta p_c, \delta p_f$, and $\delta \theta$ as the independent variables in our thermomechanical theory, we define the dependent variables $\delta e \equiv \delta V/V$, $\delta \zeta = (\delta V_\phi - \delta V_f)/V$, and $\delta s$, which are respectively the total volume dilatation, the increment of fluid content, and the increment of entropy. Introducing the combination of moduli $\sigma = 1 - K/K_s$, we find the general relations may be expressed by

\[
\begin{pmatrix}
\delta e \\
-\delta \zeta \\
\delta s
\end{pmatrix} =
\begin{pmatrix}
1/K & -\sigma/K & 3\alpha \\
-\sigma/K & 1/M + \alpha^2/K & 3\phi(\alpha_f - \alpha_\phi) \\
3\alpha & 3\phi(\alpha_f - \alpha_\phi) & [\phi_f (f) + (1 - \phi) c_p]/\theta_0
\end{pmatrix}
\begin{pmatrix}
-\delta p_c \\
-\delta p_f \\
\delta \theta
\end{pmatrix}.
\]

(4)
The constant $M$ is related to the other moduli by
\[
\frac{1}{M} = \frac{\sigma}{K_s} + \phi \left( \frac{1}{K_f} - \frac{1}{K_\phi} \right). \tag{5}
\]

The heat capacity at constant pressure for the fluid is $c_p^{(f)}$ and for the composite frame is $c_p$, while the ambient temperature is $\theta_0$. The first equation in (4) is just a restatement of (1). The second equation follows immediately from (2) and (3). The third equation follows from the definition of the entropy\(^8,^9\) and reciprocity, since the matrix in (4) must be both symmetric and nonnegative.

Now the unjacketed modulus can be related to the thermal expansion coefficient and the constituents’ properties. Suppose a composite porous medium is composed of two types of porous solid (A,B) occupying volume fractions $\nu_A = V^{(A)}/V$ and $\nu_B = V^{(B)}/V$, respectively. The porosities of these two constituents are $\phi^{(A)}$ and $\phi^{(B)}$, at least one of which must be nonzero and composed of connected pores. The drained frame moduli of the constituents are $K^{(A)}$ and $K^{(B)}$, while the material (or grain) moduli are $K_m^{(A)}$ and $K_m^{(B)}$. The thermal expansion coefficients of the constituent grains (and therefore also of the frames and pores) are $\alpha^{(A)}$ and $\alpha^{(B)}$. The heat capacities at constant pressure for the constituents are $c_p^{(A)}$ and $c_p^{(B)}$. These two constituents may not fill up the entire volume, so the volume fraction of cracks or voids is given by $\nu_C = 1 - \nu_A - \nu_B$. Consider the *gedanken* experiment in the unjacketed, nonisothermal configuration ($\delta p_f = 0$, $\delta \theta \neq 0$) such that the relative change in the volumes $V^{(A)}/V$, $V^{(B)}/V$ of the constitutents are the same and therefore also equal\(^3\) to that of the total volume $V$. Then, we have the set of equalities

\[
-\frac{\delta V}{V} = \frac{\delta p_f}{K_s} - 3\alpha \delta \theta
= \frac{\delta p_f}{K_m^{(A)}} - 3\alpha^{(A)} \delta \theta
= \frac{\delta p_f}{K_m^{(B)}} - 3\alpha^{(B)} \delta \theta. \tag{6}
\]

It follows that these equalities are satisfied if the changes of these fields have the ratio

\[
3 \frac{\delta \theta}{\delta p_f} = \frac{1/K_m^{(A)} - 1/K_m^{(B)}}{\alpha^{(A)} - \alpha^{(B)}} = \frac{1/K_s - 1/K_m^{(B)}}{\alpha - \alpha^{(B)}}
= \frac{1/K_m^{(A)} - 1/K_s}{\alpha^{(A)} - \alpha}. \tag{7}
\]

These relations determine $K_s$ in terms of $\alpha$ together with the constituents’ moduli $K_m^{(A)}$, $K_m^{(B)}$ and thermal expansion coefficients $\alpha^{(A)}$, $\alpha^{(B)}$. If the bulk moduli of the constituents are the same so $K_m^{(A)} = K_m^{(B)}$, then clearly the unjacketed modulus satisfies $K_s = K_m^{(A)}$ regardless of the values of the thermal expansion coefficients.

For the combination of $\delta p_f$ and $\delta \theta$ given by (7), the porosity of the composite does not change. In fact, changes in $p_f$ and $\theta$ do not induce changes in porosity for either constituent
and, since the overall deformation takes the form of uniform swelling or shrinking, \( \phi \) is constant. Thus,

\[
\frac{\delta \phi}{\phi} = \left( \frac{1}{K_\phi} - \frac{1}{K_s} \right) \delta p_f - 3 \left( \alpha_\phi - \alpha \right) \delta \theta \equiv 0.
\]  

(8)

Combining the result (7) with (8), we find

\[
\frac{1}{K_\phi} = \frac{1}{K_s} + \left( \alpha_\phi - \alpha \right) \left( \frac{1/K_m^{(A)} - 1/K_m^{(B)}}{1/K_m^{(A)} - 1/K_m^{(B)}} \right).
\]  

(9)

In the limit of equal constituent bulk moduli, it is again clear that \( K_\phi = K_s = K_m^{(A)} = K_m^{(B)} \) regardless of the values of the \( \alpha \). The result (9) could also have been obtained by noting that \( \delta \zeta \) in (4) equals the volume average of the fluid increments in the three types of constituents. Although instructive, this approach is much less efficient at producing the desired result (9) than the derivation presented here.

The increment of entropy \( \delta s \) may also be computed as the average of the constituent entropies. Using this approach, we find that the effective heat capacity \( c_p \) of the porous frame is determined by

\[
c_p = \langle c_p \rangle_s + 9 \theta_0 \left[ (\alpha - \phi_\alpha)/(1 - \phi) - \langle \alpha \rangle_s \right] \left( \frac{\alpha_\phi^{(A)} - \alpha_\phi^{(B)}}{1/K_m^{(A)} - 1/K_m^{(B)}} \right),
\]  

(10)

where the average \( \langle \cdot \rangle_s \) is over the solid volume \( s \), for example,

\[
\langle c_p \rangle_s = \left[ v_A (1 - \phi^{(A)}) c_p^{(A)} + v_B (1 - \phi^{(B)}) c_p^{(B)} \right] / (1 - \phi).
\]  

(11)

Note that (10) reduces correctly to the result of Rosen and Hashin\textsuperscript{10} when the porosity \( \phi \to 0 \).

Various other exact results may be obtained using standard arguments from thermodynamics. For example, consider the limit of constant total volume (\( \delta \varepsilon = 0 \)) when the porous frame is drained of fluid. Then, it is easy to show that the heat capacity at constant volume is given by \( c_v = c_p - 9\alpha^2 \theta/\left(1 - \phi \right) \), reducing to the standard result when \( \phi \to 0 \). This expression and the equivalent results for the constituent heat capacities \( c_v^{(A)} \) and \( c_v^{(B)} \) may be used to eliminate the \( c_p \)'s in (11), thereby producing an exact expression for \( c_v \) in terms of constituent properties. Similarly, considering the adiabatic (\( \delta s = 0 \)) limit when the frame is drained of fluid, shows that the adiabatic bulk modulus of the porous frame is \( K_a = K c_p / c_v \). Once exact results are available for all these constants, then the Gr"uneisen parameter \( \gamma = 3\alpha K/c_v \) may also be computed for the composite porous medium.

Two other results may be obtained in the undrained (and confined \( \delta \zeta = 0 \)), isothermal (\( \delta \theta = 0 \)) limit. The undrained bulk modulus\textsuperscript{4} is easily shown to be \( K_u = K / \left(1 - \sigma B \right) \) and the undrained thermal expansion coefficient\textsuperscript{7} is \( \alpha_u = \alpha + (\alpha_f - \alpha_\phi) B \), where the factor \( B \), given by \( B = \sigma M / \left(K + \sigma^2 M \right) \), is known as Skempton's coefficient.\textsuperscript{11}

Using data from Refs. 12–14, some examples of typical values of the bulk moduli and thermal expansion coefficients of minerals and metals are presented in Tables I and II. These values are used to evaluate the inverse of the ratio in (7) for some pairs of minerals in Table III. We see that this factor can have either sign. Recalling that 1 GPa = 1 kJ/cm\(^3\) and assuming that the
difference \((\alpha_\phi - \alpha) \approx \pm 5 \times 10^{-7} \circ K^{-1}\), the correction to the pore bulk modulus \((1/K_\phi - 1/K_s)\) can be negligible or it can be of the same order of magnitude as the unjacketed compressibility \(1/K_s\). Thus, the importance of this correction term is strongly problem dependent. On the other hand, the correction to the specific heat \((c_p - (c_p)_s)\) is of about the same order as the difference \((c_p - c_s)\) and therefore generally negligible.

It is difficult to make any further quantitative progress until some of the remaining unknowns in the equations such as \(\alpha, \alpha_\phi\), or \(K_\phi\) have been measured.

The results (7), (9), and (10) apply generally to two-component composite porous media with or without additional voids or cracks present. The authors' earlier exact results\(^3\) for \(K_s\) and \(K_\phi\) in terms of the frame and grain moduli of the components are valid only when these constituents are volume filling, so no additional voids or cracks were allowed. Thus, both sets of formulas are valid in the absence of extra voids and cracks and, therefore, additional relations between the various bulk moduli and the thermal expansion coefficients follow easily from the results presented here in this special case.

Another advantage of the new formulas is that the key ratio found in (7) depends only on material constants \(K_m\) and \(\alpha\) (that are commonly tabulated for minerals, metals, etc.) and—most importantly—have no dependence on the porosity. By contrast, the earlier formulas\(^3\) depend on the frame moduli of the porous constituents, which depend implicitly on the porosities and therefore are more difficult to tabulate.

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References


Table I. Density, isothermal bulk moduli, linear thermal expansion coefficients, and heat capacities of various minerals at 20°C. Data from refs. 12 and 13.

<table>
<thead>
<tr>
<th>Mineral</th>
<th>Formula</th>
<th>$\rho$ (g/cm$^3$)</th>
<th>$K_m$ (GPa)</th>
<th>$\alpha$ ($^{\circ}$K$^{-1}$)</th>
<th>$c_p$ (J/g$^{\circ}$K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Corundum</td>
<td>Al$_2$O$_3$</td>
<td>3.987</td>
<td>263.2</td>
<td>$5.4 \times 10^{-6}$</td>
<td>0.775</td>
</tr>
<tr>
<td>Lime</td>
<td>CaO</td>
<td>3.345</td>
<td>113.6</td>
<td>12.7</td>
<td>0.751</td>
</tr>
<tr>
<td>Microcline</td>
<td>KAlSi$_3$O$_8$</td>
<td>2.560</td>
<td>52.1</td>
<td>5.3</td>
<td>0.727</td>
</tr>
<tr>
<td>$\alpha$-Quartz</td>
<td>SiO$_2$</td>
<td>2.648</td>
<td>37.1</td>
<td>11.7</td>
<td>0.742</td>
</tr>
</tbody>
</table>

Table II. Density, isothermal bulk moduli, linear thermal expansion coefficients, and specific heats of various metals at 25°C and a pressure of 100 kPa. Data from refs. 13 and 14.

<table>
<thead>
<tr>
<th>Metal</th>
<th>Formula</th>
<th>$\rho$ (g/cm$^3$)</th>
<th>$K_m$ (GPa)</th>
<th>$\alpha$ ($^{\circ}$K$^{-1}$)</th>
<th>$c_p$ (J/g$^{\circ}$K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Iron</td>
<td>Fe</td>
<td>7.87</td>
<td>166.7</td>
<td>11.8</td>
<td>0.449</td>
</tr>
<tr>
<td>Nickel</td>
<td>Ni</td>
<td>8.91</td>
<td>185.2</td>
<td>13.4</td>
<td>0.444</td>
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<tr>
<td>Copper</td>
<td>Cu</td>
<td>8.93</td>
<td>133.3</td>
<td>16.5</td>
<td>0.385</td>
</tr>
<tr>
<td>Silver</td>
<td>Ag</td>
<td>10.50</td>
<td>99.0</td>
<td>18.9</td>
<td>0.235</td>
</tr>
</tbody>
</table>

Table III. Ratios of fluid pressure and temperature change [see Eq. (7)] resulting in uniform expansion or contraction for various pairs of minerals. Values used are those displayed in Tables I and II.

<table>
<thead>
<tr>
<th>Mineral Pairs</th>
<th>$\frac{1}{\delta_p/\delta \theta}$ (J/cm$^3$-$^{\circ}$K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SiO$_2$/Al$_2$O$_3$</td>
<td>0.272</td>
</tr>
<tr>
<td>SiO$_2$/CaO</td>
<td>-0.055</td>
</tr>
<tr>
<td>SiO$_2$/KAlSi$_3$O$_8$</td>
<td>0.825</td>
</tr>
<tr>
<td>Cu/Ag</td>
<td>-0.923</td>
</tr>
<tr>
<td>Fe/Ni</td>
<td>-2.592</td>
</tr>
<tr>
<td>Ni/Cu</td>
<td>1.475</td>
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