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On implicit constitutive theories for fluids

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We consider generalizations of fluid models wherein the fluid is assumed to be incompressible, but with the viscosity depending on the pressure. We show that a natural setting for the development of such models is a class of implicit constitutive relations, which, in addition to the fluid model described here, provides a means for developing other complex models for viscoelastic fluids which cannot be set within the ambit of classical explicit constitutive relations for the stress in terms of the histories of appropriate kinematical variables.

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1. Introduction

Constitutive expressions for the stress within the context of classical continuum mechanics such as those for the linearized response of solids due to Hooke and Navier, and for the linear response of fluids due to Newton, Navier, Poisson, St. Venant and Stokes provide explicit relationships for the stress in terms of appropriate kinematical quantities and the density. In contrast, many constitutive relations for inelastic and viscoelastic fluids are implicit relations. In this short paper, we shall discuss a generalization of the classical incompressible Navier–Stokes fluid, as envisioned by Stokes (1845), that leads to implicit constitutive relations.

In his celebrated paper on the constitutive response of fluids, Stokes (1845) recognized that the viscosity of a fluid could depend on the pressure. This is evident from his remark "If we suppose μ to be independent of the pressure also, and substitute . . . " and his comment soon afterward "Let us now consider in what cases it is allowable to suppose μ to be independent of the pressure. It has been concluded by Du Buat from his experiments on the motion of water in pipes and canals, that the total retardation of the velocity due to friction is not increased by increasing the pressure . . . I shall therefore suppose that for water, and by analogy for other incompressible fluids, μ is independent of the pressure". His comment clearly implies that only in special circumstances is the viscosity independent of the pressure. While flows in canals and pipes under normal conditions do not seem to warrant the inclusion of the dependence of the viscosity on the pressure, there are several other situations where one needs to take this dependence into account, even in the case of incompressible liquids. Of course, incompressibility is an idealization and no body is truly incompressible. When the changes in the density are 'sufficiently' small, we approximate the fluid as being incompressible. This is indeed the case in applications such as elastohydrodynamics (see Szeri 1998) wherein the variations in the pressure and the viscosity are significant, while the variation in the density is insignificant.

Barus (1893) proposed the following exponential relationship between viscosity and pressure:

$$\mu = \mu_0 \exp(\alpha p),$$

where α has units Pa^{-1} and p is expressed in Pa. This equation works well up to 500 MPa but has to be modified at much greater pressures. These modifications do not significantly change the quantitative nature of the variations; the viscosity in fact rises even more sharply than predicted by Barus' equation (see Bair & Koptte 2003, figure 1). We shall now use Barus' equation to get a rough estimate of the variation in the viscosity with pressure for common organic liquids. For Naphthalemic mineral oil α has been determined experimentally to be $26.5\,\mathrm{GPa}^{-1}$ at $20\,^{\circ}\mathrm{C}$, $23.4\,\mathrm{GPa}^{-1}$ at $40\,^{\circ}\mathrm{C}$, $20\,\mathrm{GPa}^{-1}$ at $60\,^{\circ}\mathrm{C}$ and $16.4\,\mathrm{GPa}^{-1}$ at $80\,^{\circ}\mathrm{C}$ (see Högland 1999). Thus a change of pressure from 0.1 GPa to 1.0 GPa at $60\,^{\circ}\mathrm{C}$ leads to a change in the viscosity of 4.85×10^8 %! The density on the other hand changes according to the relation (see Dowson-Higginson 1966)

$$\rho = \rho_0 \left[1 + \frac{0.6p}{1 + 1.7p} \right].$$

Thus, the change in density is merely 16 %. While such a change in density will need to be taken into account if one is interested in depicting the response very accurately, in most applications one can ignore the density change and model the fluid as incompressible. For instance the percentage change in the density when the pressure changes from 2 to 3 GPa is approximately 3.5 %. In fact, experiments also show that the changes in density due to changes in pressure at high pressures is indeed negligible.

Andrade (1930) suggested the following dependence of the viscosity on pressure, density and temperature:

$$\mu(p, \rho, \theta) = A\rho^{1/2} \exp\left((p + \rho r^2) \frac{s}{\theta} \right), \tag{1}$$

where ρ denotes the density, θ the temperature, p the pressure, and r, s and A are constants. References to much of the literature concerning the pressure dependence of the viscosity of fluids prior to 1931 can be found in the magisterial treatise by Bridgman (1931). The ubiquity of dependence of viscosity on pressure, for liquids, is made amply apparent by many of the titles of the papers written by authors such as Bridgman, e.g. "The effect of pressure on the viscosity of forty-three pure liquids" (see Bridgman 1926). There has been a considerable amount of work on this subject since then and references to the relevant literature can be found in Szeri (1998) and Hron, Malek & Rajagopal (2001).

Saal & Koens (1933) assumed that the viscosity of asphaltic bitumen depended on both the shear stress and normal stress, i.e. they had a truly implicit constitutive theory, and Bingham & Stephens (1934) investigated the effect of pressure on the "fluidity" of bodies (see Murali Krishnan & Rajagopal (2003) for a discussion of the relevant issues).

Recently, Rajagopal (2003) has discussed the general structure of a variety of implicit constitutive theories. Here, we study implicit constitutive theories specifically within the context of fluids by giving more structure and specificity to the previous work.

2. Preliminary remarks

Consider the constitutive relation for an incompressible liquid that is given by

$$\boldsymbol{T} = -p\mathbf{1} + 2\mu(p, \theta)\,\boldsymbol{D}, \tag{3}$$

where $\boldsymbol{D}$ is the symmetric part of the velocity gradient and p is referred to as the pressure and θ denotes the temperature.

Now, since the fluid is incompressible it can only undergo isochoric motions and thus

$$\operatorname{div} \boldsymbol{v} = \operatorname{tr} \boldsymbol{D} = 0. \tag{4}$$

Thus, the pressure p is the mean normal stress given by

$$p = -\tfrac{1}{3} \operatorname{tr} \boldsymbol{T}.$$

In general, in incompressible nonlinear fluids the Lagrange multiplier that enforces the constraint of incompressibility is not the mean normal stress. It thus follows from (3) and (4) that

$$\boldsymbol{T} = \tfrac{1}{3}(\operatorname{tr} \boldsymbol{T})\mathbf{1} + 2[\hat{\mu}(\operatorname{tr} \boldsymbol{T}, \theta)]\boldsymbol{D}. \tag{5}$$

Let us consider a generalization of (5), namely a fluid whose stress is given by

$$\boldsymbol{T} = \tfrac{1}{3}(\operatorname{tr} \boldsymbol{T})\mathbf{1} + 2[\hat{\mu}(\operatorname{tr} \boldsymbol{T}, |\boldsymbol{D}|^2, \theta)]\boldsymbol{D}. \tag{6}$$

We notice that (6) is not an explicit relation (and neither is (5)) for the stress as a function of $\boldsymbol{D}$ but it is an implicit relation of the form

$$\boldsymbol{f}(\boldsymbol{T}, \boldsymbol{D}, \theta) = \mathbf{0}. \tag{7}$$

The Cauchy stress $\boldsymbol{T}$ in a compressible Navier–Stokes fluid is related to the symmetric part of the velocity gradient through

$$\boldsymbol{T} = -p(\rho, \theta)\mathbf{1} + [\lambda(\rho, \theta) \operatorname{tr} \boldsymbol{D}]1 + 2\mu(\rho, \theta)\boldsymbol{D}. \tag{8}$$

In general, the pressure p (given by an equation of state) and the material moduli λ and μ will depend on temperature. In the case of the classical incompressible Navier–Stokes fluid, the Cauchy stress takes the form

$$\boldsymbol{T} = -p\mathbf{1} + 2\mu(\theta)\, \boldsymbol{D}, \tag{9}$$

where $-p\mathbf{1}$ is the indeterminate part of the stress due to the constraint of incompressibility (i.e. the constraint stress) and μ is a constant. The model (4) cannot be obtained by merely taking the limit of (3); in classical continuum mechanics it follows from enforcing the constraint (7) and requiring that the constraint stress does no work. Truesdell & Noll (1992) make such an assumption for the class of materials that also includes viscoleastic materials with memory as a special subclass. They observe “The stress $\boldsymbol{T}$ at time t is determined by the history $\boldsymbol{F}^t(s)$ of the deformation gradient only to within a stress $\boldsymbol{N}$ that does no work in any motion satisfying the constraint”. This assumption that the constraint stress does no work can be traced back to the work of D’Alembert and Bernoulli. Gauss (1829) recognized that such a requirement of worklessness was not valid in general for the motion of rigid bodies and he proposed an alternative requirement that the constraint force be the minimum force to enforce the constraint (see Rajagopal (2003) for a detailed discussion of related issues such as the nature of constraint reactions). Recently, Rajagopal & Srinivasa (2005) have shown that it is unnecessary within the context of continua to appeal to the assumption that the constraint stress is workless and they develop a purely geometrical method for describing the constraint response that is completely in keeping with the work of Gauss (1829).

The standard procedure in classical mechanics is to split the Cauchy stress $\boldsymbol{T}$ into

$$\boldsymbol{T} = \boldsymbol{T}_c + \boldsymbol{T}_E, \tag{10}$$

where $\boldsymbol{T}_c$, the constraint reaction (constraint stress), is assumed to not depend on the state variables (in the case of the classical fluid the velocity gradient) and $\boldsymbol{T}_E$ the 'extra' stress which is constitutively prescribed, but is assumed to not depend on the constrained part $\boldsymbol{T}_c$. The further assumption that $\boldsymbol{T}_c$ does no work implies that

$$\boldsymbol{T}_c \cdot \boldsymbol{D} = 0 \text{ whenever } \operatorname{tr} \boldsymbol{D} = (\mathbf{1} \cdot \boldsymbol{D}) = \operatorname{div} \boldsymbol{v} = 0. \tag{11}$$

This immediately leads to

$$\boldsymbol{T}_c = \phi \mathbf{1} \tag{12}$$

and one usually uses the symbol $p = -\phi$ in expressing (12). Importantly, $\boldsymbol{T}_E$ cannot depend on p, and thus quantities such as the viscosity cannot depend on the pressure. It is also important to note that the above procedure would be inapplicable if the constraint were nonlinear in $\boldsymbol{D}$, say

$$\operatorname{tr} \boldsymbol{D}^3 = 0. \tag{13}$$

In any event, the standard procedure leads to the material function not depending on the constraint.

As the standard procedure will not lead to the model (3), which is also subject to the constraint (4), we now consider an alternative procedure that not only leads to the model (3) but also to various generalizations of the model. In order to do this, we will have to consider a general class of implicit constitutive relations.

3. Implicit constitutive models

Let us consider an implicit relation of the form (7), i.e. between the stress and the symmetric part of the velocity gradient. It then follows that

$$\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{T}} \dot{\boldsymbol{T}} + \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{D}} \dot{\boldsymbol{D}} + \frac{\partial \boldsymbol{f}}{\partial \theta} \dot{\theta} = 0, \tag{14}$$

where $\partial \boldsymbol{f}/\partial \boldsymbol{T}$ and $\partial \boldsymbol{f}/\partial \boldsymbol{D}$ are fourth-order tensors and $\partial \boldsymbol{f}/\partial \theta$ a second-order tensor, the dot denoting the material time derivative. Models of the form (14) may not be generally frame-indifferent, but this can be easily rectified by introducing frame-indifferent time derivatives. On the other hand, one can easily construct models of the form (14) that are frame indifferent and the models discussed below are examples of such frame-indifferent models. We could also start with models of the form

$$[\boldsymbol{A}(\boldsymbol{T}, \boldsymbol{D}, \theta)]\dot{\boldsymbol{T}} + [\boldsymbol{B}(\boldsymbol{T}, \boldsymbol{D}, \theta)]\dot{\boldsymbol{D}} + \boldsymbol{C}(\boldsymbol{T}, \boldsymbol{D}, \theta)\dot{\theta} = 0, \tag{15}$$

where $\boldsymbol{A}$ and $\boldsymbol{B}$ are fourth-order tensors and $\boldsymbol{C}$ a second order tensor. While the class of models defined through (15) is larger, in one sense, than that defined through (7) in that not all models belonging to (15) belong to (7) as (15) may not be integrable, we note that (15) requires the stress $\boldsymbol{T}$ and the tensor $\boldsymbol{D}$ have time derivatives while (7) makes no such restriction. However, we shall be interested in sufficiently smooth functions $\boldsymbol{T}$ and $\boldsymbol{D}$, as for that class of functions (15) is more general than (7). Given a model, say equation (6), since it can always be expressed in the form (7), we can further express it in the form (15) by merely taking its derivative. Henceforth, for the sake of simplicity, we shall ignore temperature; however it is easy to incorporate it into the theory.

Suppose

$$\left.\begin{aligned} \boldsymbol{A}(\boldsymbol{T},\boldsymbol{D}) &:= \left\{\mathfrak{I} - \tfrac{1}{3}\mathbf{1}\otimes\mathbf{1} - 2[\mu'(\operatorname{tr}\boldsymbol{T})](\boldsymbol{D}\otimes\mathbf{1})\right\}, \qquad (16)\\ \boldsymbol{B}(\boldsymbol{T},\boldsymbol{D}) &:= \{2[\mu'(\operatorname{tr}\boldsymbol{T})]\mathfrak{I}\},\ \frac{\partial \boldsymbol{f}}{\partial\theta} = 0, \qquad (17)\end{aligned}\right\}$$

where $\mathfrak{I}$ denotes the fourth-order identity tensor and μ is a sufficiently smooth function of $\operatorname{tr}\boldsymbol{T}$, and the prime denotes differentiation with respect to the argument. The symbol $\otimes$ stands for the tensor product operation between two second-order tensors. Thus, $\boldsymbol{D}\otimes\mathbf{1}$ and $\mathbf{1}\otimes\mathbf{1}$ are fourth-order tensors.

Since we are interested in describing incompressible fluids, we shall require that (4) is met.

It follows from (15), (16) and (17) that

$$\dot{\boldsymbol{T}} - \tfrac{1}{3}(\mathbf{1}\cdot\dot{\boldsymbol{T}})\mathbf{1} - 2[\mu'(\operatorname{tr}\boldsymbol{T})](\boldsymbol{D}\otimes\boldsymbol{T})\dot{\boldsymbol{T}} = \{2[\mu(\operatorname{tr}\boldsymbol{T})]\mathfrak{I}\}\dot{\boldsymbol{D}}. \qquad (18)$$

Equation (18) can be re-written as

$$\dot{\boldsymbol{T}} = \tfrac{1}{3}(\operatorname{tr}\dot{\boldsymbol{T}})\mathbf{1} + 2[\mu'(\operatorname{tr}\boldsymbol{T})](\operatorname{tr}\dot{\boldsymbol{T}})\boldsymbol{D} + 2[\mu(\operatorname{tr}\boldsymbol{T})]\dot{\boldsymbol{D}}, \qquad (19)$$

which can be integrated to yield

$$\boldsymbol{T} = \tfrac{1}{3}(\operatorname{tr}\boldsymbol{T})\mathbf{1} + 2[\mu(\operatorname{tr}\boldsymbol{T})]\boldsymbol{D} + \boldsymbol{T}_0, \qquad (20)$$

where $\boldsymbol{T}_0$ is some constant symmetric stress tensor.

If we require that the stress be purely spherical when $\boldsymbol{D} = \mathbf{0}$, we obtain

$$\boldsymbol{T} = \tfrac{1}{3}(\operatorname{tr}\boldsymbol{T})\mathbf{1} + 2[\mu(\operatorname{tr}\boldsymbol{T})]\boldsymbol{D}. \qquad (21)$$

We notice that (21) automatically meets the constraint (4). We thus do not need to enforce the constraint of incompressibility by using a Lagrange multiplier as is done within the classical context.

Let us define

$$p := -\tfrac{1}{3}\operatorname{tr}\boldsymbol{T}. \qquad (22)$$

Then

$$\boldsymbol{T} = -p\mathbf{1} + 2\hat{\mu}(p)\boldsymbol{D}. \qquad (23)$$

Next, let us suppose that we are given a function where

$$\mu = \mu(\operatorname{tr}\boldsymbol{T}, |\boldsymbol{D}|^2.) \qquad (24)$$

Consider

$$\boldsymbol{A}(\boldsymbol{T},\boldsymbol{D}) = \left\{\mathfrak{I} - \tfrac{1}{3}\mathbf{1}\otimes\mathbf{1} - 2\frac{\partial\mu}{\partial(\operatorname{tr}\boldsymbol{T})}(\boldsymbol{D}\otimes\mathbf{1})\right\}, \qquad (25)$$

and

$$\boldsymbol{B}(\boldsymbol{T},\boldsymbol{D}) - \ = -\left\{2\mu\mathfrak{I} + 4\frac{\partial\mu}{\partial(|\boldsymbol{D}|^2)}\boldsymbol{D}\otimes\boldsymbol{D}\right\}. \qquad (26)$$

It then follows from (15), (25) and (26) that

$$\dot{\boldsymbol{T}} - \tfrac{1}{3}(\operatorname{tr}\dot{\boldsymbol{T}})\mathbf{1} - 2\frac{\partial\mu}{\partial(\operatorname{tr}\boldsymbol{T})}(\operatorname{tr}\dot{\boldsymbol{T}})\boldsymbol{D} = 2\mu\dot{\boldsymbol{D}} + 4\frac{\partial\mu}{\partial(|\boldsymbol{D}|^2)}(\boldsymbol{D}\cdot\dot{\boldsymbol{D}})\boldsymbol{D}, \qquad (27)$$

which can be re-written as

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\boldsymbol{T} - \tfrac{1}{3}(\operatorname{tr}\boldsymbol{T})\mathbf{1}\right] = \frac{\mathrm{d}}{\mathrm{d}t}\{2[\mu(\operatorname{tr}\boldsymbol{T}, |\boldsymbol{D}|^2)]\boldsymbol{D}\}. \qquad (28)$$

This can be integrated to yield

$$\boldsymbol{T} = \tfrac{1}{3}(\mathrm{tr}\,\boldsymbol{T})\mathbf{1} + 2[\mu(\mathrm{tr}\,\boldsymbol{T}, |\boldsymbol{D}|^2)]\boldsymbol{D} + \boldsymbol{T}_0, \tag{29}$$

where $\boldsymbol{T}_0$ is a constant tensor. Once again requiring that when the fluid is at rest we have a spherical state of stress leads to

$$\boldsymbol{T} = \tfrac{1}{3}(\mathrm{tr}\,\boldsymbol{T})\mathbf{1} + 2[\mu(\mathrm{tr}\,\boldsymbol{T}, |\boldsymbol{D}|^2)]\boldsymbol{D}. \tag{30}$$

We can obtain further generalizations of the Navier–Stokes model by considering other forms for $\boldsymbol{A}(\boldsymbol{T}, \boldsymbol{D})$ and $\boldsymbol{B}(\boldsymbol{T}, \boldsymbol{D})$.

Let us consider the implications of assuming that $\boldsymbol{f}$ defined through the relation (7) is an isotropic function of the tensors $\boldsymbol{T}$ and $\boldsymbol{D}$. Then

$$\boldsymbol{f}(\boldsymbol{QTQ}^T, \boldsymbol{QDQ}^T) = \boldsymbol{Qf}(\boldsymbol{T}, \boldsymbol{D})\boldsymbol{Q}^T \quad \forall \boldsymbol{Q} \in \dot{O} \tag{31}$$

where $\dot{O}$ denotes the set of all orthogonal transformations. It then follows that (see Spencer 1975)

$$\alpha_0\mathbf{1} + \alpha_1\boldsymbol{T} + \alpha_2\boldsymbol{D} + \alpha_3\boldsymbol{T}^2 + \alpha_4\boldsymbol{D}^2 + \alpha_5(\boldsymbol{DT} + \boldsymbol{TD}) + \alpha_6(\boldsymbol{T}^2\boldsymbol{D} + \boldsymbol{DT}^2) + \alpha_7(\boldsymbol{TD}^2 + \boldsymbol{D}^2\boldsymbol{T}) + \alpha_8(\boldsymbol{T}^2\boldsymbol{D}^2 + \boldsymbol{D}^2\boldsymbol{T}^2) = \mathbf{0}, \tag{32}$$

where the material functions $\alpha_i, i = 0, \ldots, 8$, depend on the invariants

$$\mathrm{tr}\,\boldsymbol{T}, \mathrm{tr}\,\boldsymbol{D}, \mathrm{tr}\,\boldsymbol{T}^2, \mathrm{tr}\,\boldsymbol{D}^2, \mathrm{tr}\,\boldsymbol{T}^3, \mathrm{tr}\,\boldsymbol{D}^3, \mathrm{tr}\,(\boldsymbol{TD}), \mathrm{tr}\,(\boldsymbol{T}^2\boldsymbol{D}), \mathrm{tr}\,(\boldsymbol{D}^2\boldsymbol{T}), \mathrm{tr}\,(\boldsymbol{D}^2\boldsymbol{T}^2). \tag{33}$$

To include the effect of density and temperature is trivial: all that is necessary is to include them in the list of quantities listed in (33) on which the material functions depend. We immediately recognize that (21) and (29) as well as the classical incompressible Navier–Stokes model are all special cases of (32). Now, regarding representation (29) the fact that $\boldsymbol{T}$ and $\boldsymbol{D}$ are related through (7) and that the density does not feature explicitly in the relationship does not mean that the body under consideration has to meet $\mathrm{tr}\,\boldsymbol{D} = 0$.

When we consider fluid models of the form (32) and (33), if

$$\alpha_0 = +\left(\tfrac{1}{3}\mathrm{tr}\,\boldsymbol{T}\right), \quad \alpha_1 \equiv 1, \quad \alpha_2 = -\mu(\mathrm{tr}\,\boldsymbol{T}) \tag{34}$$

and all the other α_i are identically zero, we obtain the model (23). Such a constitutive assumption automatically implies that the body under consideration is incompressible as it always meets the constraint (4), i.e. the special choice of α_0, α_1 and α_2 guarantees that the fluid is incompressible and that the stress is given by (3). We do not need to necessarily enforce the constraint via Lagrange multipliers or require that the constraint stress is workless while working with these implicit models. This point cannot be overemphasized.

Further generalizations can be achieved by selecting implicit relations of the form

$$\boldsymbol{f}\left(\boldsymbol{T}, \dot{\boldsymbol{T}}, \ldots \overset{(n)}{\boldsymbol{T}}, \boldsymbol{D}, \dot{\boldsymbol{D}}, \ldots \overset{(n)}{\boldsymbol{D}}\right) = \mathbf{0}, \tag{35}$$

where the superscript (n) stands for n material time derivatives. Such models include many of the rate-type models that are used to describe viscoelastic fluids.

4. Concluding remarks

Most models for fluids (solids) assume that either the material moduli that characterize them are constants or that they depend on the temperature and kinematical quantities such as the shear rate (shear), etc. When considering materials that satisfy constraints such as incompressibility, the material moduli are not allowed to depend on the constraint response and this is a consequence of a procedure that has now become quite standard in mechanics; that of requiring that the constraint stresses do no work. Such an assumption precludes the possibility of the viscosity of an incompressible fluid depending on the pressure. Here, we have discussed a more generalized implicit constitutive framework for the modelling of materials that allows for fluid models wherein the viscosity depends on the pressure; more generally the material moduli to depend on the Lagrange multiplier that enforces the constraint. A further generalization of the framework proposed here would allow one to construct models for turbulent flows wherein the material functions can depend on the invariants associated with the stresses and their fluctuations as opposed to allowing them to only depend on the fluctuations in the velocity gradients.

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