

Aspects of the thermodynamic stability of fibre suspension flows

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Abstract

We examine the circumstances under which the constitutive equations for fibre suspension flows are consistent with the second law of thermodynamics, and the conditions under which fibre suspension flows are stable, in the energetic sense. The constitutive model investigated is that based on the use of orientation tensors, and these issues are examined in the context of a selection of closure approximations: the linear and quadratic closures, a rule due to Hinch and Leal, the smooth orthotropic closure rule of Cintra and Tucker, and the natural closure of Verleye and Dupret. It is shown that, with the use of the linear closure approximation, the constitutive equations are consistent with the second law, and the flows are monotonically stable, if the particle number does not exceed $35/2$. The quadratic closure is consistent and stable, as is the natural closure, at least in the two-dimensional case. It is not possible to determine the stability or otherwise of the Hinch–Leal closure for arbitrary flows, though for biaxial elongation, a case which is known to lead to non-physical results, the closure rule is consistent with the second law of thermodynamics. The smooth orthotropic rule of Cintra and Tucker is shown not to be consistent with the second law for arbitrary flows. © 2000 Elsevier Science B.V. All rights reserved.

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1. Introduction

A currently popular constitutive model for fibre suspension flows is one in which fibres are accounted for through the introduction of second- and fourth-order orientation tensors [1,13,14]. Such models have the great advantage that the average behaviour of fibres may be treated in a deterministic manner, and without the need to solve rather complex equations for the probability density function which characterises fibre orientations.

It is necessary, in models based on orientation tensors, to make use of a closure approximation in order to express the fourth-order orientation tensor in terms of that of order two. Solutions of the resulting problems depend critically on the choice of closure rule, and while it is found that some rules are particularly well

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suited to specific flow situations, no single rule can be said to lead to accurate simulations of all flow situations.

Popular closure approximations have been those of linear and quadratic type. These, together with other approximations such as those due to Hinch and Leal [10], have been reviewed and compared by Advani and Tucker [2], who show that there is marked variation in the quality of approximations of the different closure rules studied.

In a recent study of the well-posedness of the set of equations describing fibre suspensions flows [9], Galdi and Reddy have shown that there is a close connection between stability, in the Liapounov sense, and the particle number, a parameter closely related to fibre concentration, for the case in which a linear closure approximation is used. In particular, the rest state is shown to be unstable for particle numbers exceeding $35/2$. A second result in that work is one on local existence and uniqueness of solutions, for closure rules corresponding to stable rest states.

The inherent instability asserts itself also in the behaviour of the evolution equation, in which concentration is not present as a parameter. It is shown, in a numerical study by Reddy and Mitchell [12], that whereas quadratic and hybrid closures converge rapidly to the steady state, the use of the linear closure gives rise to a transient region which is oscillatory for a relatively extended period of time.

The purpose of this contribution is to work towards a more complete picture of the stability of fibre suspension flows, by investigating thermodynamic and energetic stability for these flows, and their relationship to the choice of closure rule. The constitutive equations adopted in [9] and elsewhere are used, and the circumstances under which these equations are consistent with the second law of thermodynamics are investigated. Second, the conditions under which flows are monotonically or exponentially stable, in an energetic sense, are studied. The study focusses on a representative sample of closures: the linear and quadratic rules; a rule proposed by Hinch and Leal [10], and commonly referred to as H&L1; the smooth orthotropic closure rule due to Cintra and Tucker [3]; and the natural closure proposed by Dupret and Verleye [7]. The findings in [9] are confirmed here, in the sense that, for the quadratic closure, the constitutive equations are consistent with the second law, and are exponentially stable, while for the linear closure rule a sufficient condition is obtained: flows are consistent and stable if the particle number does not exceed $35/2$. It is not possible to determine the stability or otherwise of the Hinch–Leal closure for arbitrary flows, since the expression for dissipation is of indeterminate sign. For biaxial elongation, though, a case which is known to lead to non-physical results [2], the closure rule is consistent with the second law of thermodynamics. The smooth orthotropic rule of Cintra and Tucker is shown not to be consistent with the second law for arbitrary flows, in the sense that the dissipation may take either sign. For specific flows, though, it is possible to establish the consistency of the rule. The natural closure is shown to be consistent and stable, at least in two-dimensional situations.

In Section 2, the constitutive equations for fibre suspension flows are reviewed, and the associated initial boundary value problem is presented. Thermodynamic restrictions on the constitutive laws are investigated in Section 3, while energetic stability is the subject of Section 4.

1.1. Notation

We make use of coordinate-free notation wherever convenient, and denote vectors and tensors by bold-face letters. The scalar product of two vectors \mathbf{u} and \mathbf{v} is denoted by $\mathbf{u} \cdot \mathbf{v}$, while the corresponding product of two second-order tensors \mathbf{A} and \mathbf{B} is denoted by $\mathbf{A} : \mathbf{B}$. In index form these expressions read

$u_i v_i$ and $A_{ij} B_{ij}$, the summation convention on repeated indices being applied at all times. The magnitude of a vector \mathbf{u} and a tensor \mathbf{A} are then defined in a natural way by $|\mathbf{u}| = (\mathbf{u} \cdot \mathbf{u})^{1/2}$ and $|\mathbf{A}| = (\mathbf{A} : \mathbf{A})^{1/2}$.

2. Fibre suspension flows

We give here a brief but self-contained review of the equations governing the flow of fibre suspensions. Detailed accounts may be found, for example, in the works of Advani and Tucker [1,13,14].

2.1. Fibre suspensions

For the purposes of this investigation a fibre suspension is defined to be a viscous incompressible fluid in which is suspended a distribution of axisymmetric, rigid, and ideally massless fibres. The fibre volume fraction is denoted by h , and the fibre aspect ratio r is defined by $r = \ell/d$, where ℓ and d are respectively the fibre length and diameter.

A suspension is said to be

$$\left. \begin{array}{l} \text{dilute} \\ \text{semi-dilute} \\ \text{concentrated} \end{array} \right\} \text{if } \left\{ \begin{array}{l} hr^2 < 1 \\ 1 < hr^2 < r \\ r < hr^2 \end{array} \right. . \tag{2.1}$$

We consider dilute and semi-dilute suspensions, for which fibres have a low probability of making contact, though the fibres and the fluid motion are coupled.

The orientation of each fibre is described by a unit vector \mathbf{p} . It is unrealistic to attempt to develop a theory based on the orientation and motion of individual fibres, and a more useful approach is that of introducing a probability density function $\psi(\mathbf{p})$ whose value for a given orientation gives the probability that a fibre has that particular orientation.

The distribution function $\psi(\mathbf{p})$ provides a general description of the orientation state, and it is possible to make direct calculations of ψ for a single point in a suspension. But in continuum-based approaches for suspensions containing a realistic volume fraction of fibres, it is desirable to eliminate the probability density as a variable. This is done by first introducing the orientation tensors \mathbf{A} and \mathcal{A} ; these are respectively a second- and fourth-order tensor, defined by

$$\mathbf{A} = \langle \mathbf{p} \otimes \mathbf{p} \rangle, \tag{2.2}$$

$$\mathcal{A} = \langle \mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p} \otimes \mathbf{p} \rangle, \tag{2.3}$$

and which contain information, in an averaged sense, about the distribution of fibre orientation. Here

$$\langle f \rangle = \int f(\mathbf{p}) \psi(\mathbf{p}) \, d\mathbf{p}$$

is the averaging operator with respect to the probability distribution ψ . The second-order tensor has the properties

$$A_{ji} = A_{ij} \text{ and } A_{ii} = 1, \tag{2.4}$$

while the fourth-order tensor has the symmetry properties

$$\mathcal{A}_{ijkl} = \mathcal{A}_{jikl} = \mathcal{A}_{kijl} = \mathcal{A}_{klij}, \text{ etc.} \quad (2.5)$$

By making use of these definitions and of the equations of conservation of fibres, and of the motion of a single particle, it is possible to derive an evolution equation for the tensor \mathbf{A} : for a problem in R^n , this is given by [2]

$$\frac{D\mathbf{A}}{Dt} = (\mathbf{W}\mathbf{A} - \mathbf{A}\mathbf{W}) + \lambda(\mathbf{D}\mathbf{A} + \mathbf{A}\mathbf{D} - 2\mathcal{A}\mathbf{D}) + D_r(\mathbf{I} - n\mathbf{A}). \quad (2.6)$$

Here

$$\frac{D\mathbf{A}}{Dt} \equiv \frac{\partial \mathbf{A}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{A} \quad (2.7)$$

is the material derivative,

$$\mathbf{D} = \frac{1}{2}[\nabla\mathbf{v} + (\nabla\mathbf{v})^T] \quad (2.8)$$

is the stretching tensor,

$$\mathbf{W} = \frac{1}{2}[\nabla\mathbf{v} - (\nabla\mathbf{v})^T] \quad (2.9)$$

is the spin tensor, and

$$\lambda = \frac{r^2 - 1}{r^2 + 1} \quad (2.10)$$

is a parameter that characterises particle slenderness.

The parameter D_r represents the rotary diffusivity. We make use here of an approximation proposed by Folgar and Tucker [8], in which the rotary diffusivity can be expressed as a function of the flow through the relation

$$D_r = C_1|\mathbf{D}|, \quad (2.11)$$

where C_1 is an empirical constant known as the interaction coefficient. It should be noted that the definition of C_1 adopted here differs from that in [8] by a factor $2\sqrt{2}$; this difference has no bearing on the developments that follow.

2.2. Closure approximations

It is found that (2.7) contains the tensor \mathcal{A} ; in fact it is a feature of such evolution equations that the equation for an orientation tensor of a particular rank contains the tensor of the next (even) rank up. In order to circumvent this problem \mathcal{A} is conventionally approximated by means of what is known as a closure rule. This approximation consists of writing \mathcal{A} as a function of the second-order tensor \mathbf{A} .

The simplest closures are linear and quadratic approximations. The linear approximation \mathcal{A}^L , for incompressible fluids, is defined by

$$\mathcal{A}^L\mathbf{D} = -\frac{2}{35}\mathbf{D} + \frac{1}{7}[2\mathbf{A}\mathbf{D} + 2\mathbf{D}\mathbf{A} + (\mathbf{A} : \mathbf{D})\mathbf{I}] \quad (2.12)$$

for any symmetric second-order tensor \mathbf{D} with $\text{tr } \mathbf{D} = 0$, while the quadratic approximation \mathcal{A}^Q is defined by

$$\mathcal{A}^Q = \mathbf{A} \otimes \mathbf{A}. \tag{2.13}$$

The linear closure rule is exact for random distributions of fibres, while the quadratic closure is exact for perfectly aligned fibres.

We will later examine these two closure rules further, in the context of stability considerations. It is important, though, to expand the set of closure rules being examined, in order to arrive at a broader picture of the range of approximations in use, and of their relative merits. For this purpose we add to the linear and quadratic closures three more rules that have received some attention. These rules, the first Hinch–Leal composite closure, the Cintra–Tucker orthotropic smooth closure, and the Dupret–Verleye natural closure, are regarded as good candidates for investigation since they are simple in structure, lead to very good results in certain flow situations, but, in the case of the Hinch–Leal rule, also give rather poor, or even nonphysical results for some flows. Hinch and Leal [10] have proposed a number of different closure approximations in their study of fibre suspensions exhibiting Brownian motion. One of these, now often referred to as H&L1, is included in the present study. It is a quadratic polynomial in the components of \mathbf{A} , and is defined by

$$\mathcal{A}D = \frac{1}{5}[6\mathbf{A}D\mathbf{A} + (\mathbf{A} : \mathbf{D})(2\mathbf{I} - \mathbf{A}) - 2(\mathbf{A}^2 : \mathbf{D})\mathbf{I}]. \tag{2.14}$$

This closure rule gives accurate results for simple shear flows, and for smaller values of the interaction coefficient. It has the drawback, however, that it gives a nonphysical result in biaxial elongational flows [2].

The next example comes from an extensive study of orthotropic closure rules due to Cintra and Tucker [3]. They take as a point of departure the observation that the tensor \mathcal{A} must be orthotropic, that its principal axes coincide with those of \mathbf{A} , and that it is a function of only two of the eigenvalues of \mathbf{A} , the last property following from (2.4). These authors develop two rules, referred to as a smooth closure, and a fitted closure. The former has a simple form based on linear interpolation of the eigenvalues of \mathbf{A} , while the fitted closure rule is based on numerical solutions for the probability density function.

We confine attention to the orthotropic smooth closure. In order to describe this rule it is most convenient to follow Cintra and Tucker by writing the nonzero components of \mathcal{A} as a symmetric 6×6 matrix $\bar{\mathcal{A}}$; this matrix has the form

$$\bar{\mathcal{A}} = \begin{pmatrix} \bar{\mathcal{A}}_{11} & \bar{\mathcal{A}}_{12} & \bar{\mathcal{A}}_{13} & 0 & 0 & 0 \\ & \bar{\mathcal{A}}_{22} & \bar{\mathcal{A}}_{23} & 0 & 0 & 0 \\ & & \bar{\mathcal{A}}_{33} & 0 & 0 & 0 \\ & & & \bar{\mathcal{A}}_{23} & 0 & 0 \\ & \text{SYM} & & & \bar{\mathcal{A}}_{13} & 0 \\ & & & & & \bar{\mathcal{A}}_{12} \end{pmatrix}, \tag{2.15}$$

and has six independent components, which are related to \mathcal{A}_{ijkl} according to

$$\begin{aligned} \bar{\mathcal{A}}_{ii} &= \mathcal{A}_{iii} \quad \text{for } i = 1, 2, 3 \text{ (no sum on } i), \\ \bar{\mathcal{A}}_{ij} &= \mathcal{A}_{ijj} \quad \text{for } i, j = 1, 2, 3, i \neq j, \text{ (no sum on } i, j). \end{aligned} \tag{2.16}$$

Other nonzero components of \mathbf{A} are obtained by invoking the symmetry properties of this tensor. The elementary identity $\mathcal{A}_{ijkk} = A_{ij}$ leads to a further reduction of the number of independent components to three, through the set of equations

$$\begin{aligned}\bar{\mathcal{A}}_{11} + \bar{\mathcal{A}}_{12} + \bar{\mathcal{A}}_{13} &= A_1, \\ \bar{\mathcal{A}}_{12} + \bar{\mathcal{A}}_{22} + \bar{\mathcal{A}}_{23} &= A_2, \\ \bar{\mathcal{A}}_{13} + \bar{\mathcal{A}}_{23} + \bar{\mathcal{A}}_{33} &= A_3,\end{aligned}\tag{2.17}$$

where the eigenvalues of \mathbf{A} are written as (A_1, A_2, A_3) . The closure rule is then defined by expressing $\bar{\mathcal{A}}_{ii}$ ($i = 1, 2, 3$) as a function of two of the eigenvalues A_i . For the orthotropic smooth closure this expression takes the form [3]

$$\begin{pmatrix} \bar{\mathcal{A}}_{11} \\ \bar{\mathcal{A}}_{22} \\ \bar{\mathcal{A}}_{33} \end{pmatrix} = \begin{pmatrix} -0.15 + 1.15A_1 - 0.10A_2 \\ -0.15 + 0.15A_1 + 0.90A_2 \\ 0.60 - 0.60A_1 - 0.60A_2 \end{pmatrix},\tag{2.18}$$

and a simple computation, based on (2.17) and (2.18), leads to the expression

$$\begin{pmatrix} \bar{\mathcal{A}}_{12} \\ \bar{\mathcal{A}}_{13} \\ \bar{\mathcal{A}}_{23} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} -0.1 + 0.1A_1 + 0.6A_2 \\ 0.4 - 0.4A_1 - 0.40A_2 \\ 0.4 - 0.4A_1 - 0.40A_2 \end{pmatrix},\tag{2.19}$$

for the remaining independent components of $\bar{\mathcal{A}}$ in terms of the eigenvalues of \mathbf{A} .

The final example is due to Dupret and Verleye (see, for example, [7]). Their rule, known as the natural closure, is derived by observing first that for infinitely slender fibres and no fibre–fibre interaction, the orientation of a fibre depends only on its initial orientation and on the state of deformation. In this way it is possible to solve for $\psi(\mathbf{p})$ as a function of the initial orientation and the deformation. The resulting closure takes different forms in two and three dimensions, and an explicit representation of the natural closure is possible only in two dimensions, for which case it takes the component form

$$\mathcal{A}_{ijkl} = \frac{1}{2} \Delta S(\delta_{ij}\delta_{kl}) + S(A_{ij}A_{kl});\tag{2.20}$$

here Δ is the determinant of \mathbf{A} and S is the symmetrisation operator: in two dimensions,

$$S(B_{ijkl}) = \frac{1}{24}(B_{ijkl} + B_{ijlk} + B_{ikjl} + \dots)\tag{24 terms}.\tag{2.21}$$

Making use of (2.21) and exploiting the symmetry of δ_{ij} and A_{ij} , we find that (2.20) takes the relatively simple form

$$\mathcal{A}_{ijkl} = \frac{1}{3}[A_{ij}A_{kl} + A_{ik}A_{lj} + A_{il}A_{jk}] + \frac{1}{6}\Delta[\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{lj} + \delta_{il}\delta_{jk}].\tag{2.22}$$

2.3. Constitutive equation for the stress

Coupling of the fluid and fibre motions implies that the usual constitutive equation for the stress will be modified by terms that contain the orientation tensor. The constitutive equation for the stress is given by

$$\mathbf{T} = -p\mathbf{I} + \mathbf{S},\tag{2.23}$$

where

$$\mathbf{S} = 2\mu_1[\mathbf{D} + N_p\mathcal{A}\mathbf{D} + N_s(\mathbf{A}\mathbf{D} + \mathbf{D}\mathbf{A})]. \tag{2.24}$$

Here μ_1 contains all the isotropic contributions to viscosity while the anisotropic contributions due to the particles are represented by N_p , the particle number and N_s , the shear number. In this model rotary diffusion, which plays an important role when particles are of molecular size, is neglected.

2.4. The initial boundary value problem

We assume that the fluid occupies a bounded domain Ω with boundary Γ , and that is subjected to the action of a body force \mathbf{b} per unit mass. The fluid has mass density ρ . It is required to find the velocity field $\mathbf{v}(\mathbf{x}, t)$, the pressure $p(\mathbf{x}, t)$, and the orientation tensor field $\mathbf{A}(\mathbf{x}, t)$ which satisfy the following set of equations: conservation of momentum

$$\rho \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v} - \text{div } \mathbf{T} = \rho \mathbf{b}, \tag{2.25}$$

conservation of mass (continuity equation)

$$\text{div } \mathbf{v} = 0, \tag{2.26}$$

constitutive equation for stress

$$\mathbf{T} = -p\mathbf{I} + 2\mu_1[\mathbf{D} + N_p\mathcal{A}\mathbf{D} + N_s(\mathbf{A}\mathbf{D} + \mathbf{D}\mathbf{A})], \tag{2.27}$$

and the evolution equation for the orientation tensor

$$\frac{D\mathbf{A}}{Dt} = (\mathbf{W}\mathbf{A} - \mathbf{A}\mathbf{W}) + \lambda(\mathbf{D}\mathbf{A} + \mathbf{A}\mathbf{D} - 2\mathcal{A}\mathbf{D}) + C_1|\mathbf{D}|(\mathbf{I} - n\mathbf{A}). \tag{2.28}$$

These equations are supplemented by the boundary condition

$$\mathbf{v} = \bar{\mathbf{v}} \text{ on } \Gamma \tag{2.29}$$

and the initial conditions

$$\mathbf{v}(\mathbf{x}, 0) = \mathbf{v}_0, \quad \mathbf{A}(\mathbf{x}, 0) = \mathbf{A}_0 \text{ on } \bar{\Omega}. \tag{2.30}$$

In (2.27) and (2.28) one of the closure approximations will be used to express \mathcal{A} in terms of \mathbf{A} .

3. Thermodynamic restrictions on the constitutive equations

Since we are dealing with a purely mechanical theory, the second law of thermodynamics in this context is the requirement that the energy increase at a rate not exceeding the power expended [5]. If the free energy is denoted by Ψ , then the local form of the second law is the dissipation inequality

$$\rho \dot{\Psi} \leq \mathbf{T} : \mathbf{D}. \tag{3.1}$$

We will use the methods of Coleman, Gurtin and Noll [4,5] to investigate which restrictions, if any, are placed on the constitutive equations by the dissipation inequality. This approach has been used with great

effectiveness by Dunn and Fosdick [6] in determining the restrictions that apply to the constants appearing in the constitutive equations for fluids of second grade.

The motion of the fluid is described by the function $\mathbf{x} = \boldsymbol{\varphi}(\mathbf{X}, t)$, in which \mathbf{x} and \mathbf{X} denote reference and current position, respectively in the fluid. We assume that $\boldsymbol{\varphi}(\mathbf{X}, t)$ is smoothly invertible in its arguments, and define the deformation gradient \mathbf{F} by

$$\mathbf{F} = \nabla_{\mathbf{X}}\boldsymbol{\varphi}. \quad (3.2)$$

The inverse \mathbf{F}^{-1} of \mathbf{F} exists, and if the velocity gradient is defined by

$$\mathbf{L} = \nabla \mathbf{v}, \quad (3.3)$$

then

$$\mathbf{L} = \dot{\mathbf{F}}\mathbf{F}^{-1}. \quad (3.4)$$

For any sufficiently smooth functions \mathbf{F} and \mathbf{A} ,

$$\dot{\Psi}(\mathbf{F}, \mathbf{A}) = \Psi_{\mathbf{F}} : \dot{\mathbf{F}} + \Psi_{\mathbf{A}} : \dot{\mathbf{A}}. \quad (3.5)$$

Here $\Psi_{\mathbf{F}}$ and $\Psi_{\mathbf{A}}$ are the derivatives of Ψ with respect to \mathbf{F} and \mathbf{A} .

We now substitute (2.27), (2.28) and (3.5) in the dissipation inequality (3.1), and make use also of the incompressibility condition $\text{tr } \mathbf{D} = 0$, to obtain

$$\begin{aligned} \rho \Psi_{\mathbf{F}} \mathbf{F}^{\text{T}} : \mathbf{L} + \rho \Psi_{\mathbf{A}} : [\mathbf{A}\mathbf{W} - \mathbf{W}\mathbf{A} + \lambda(\mathbf{A}\mathbf{D} + \mathbf{D}\mathbf{A} - 2\mathbf{A}\mathbf{D}) + C_1|\mathbf{D}|(\mathbf{I} - n\mathbf{A})] \\ - 2\mu_1[\mathbf{D} + N_p\mathbf{A}\mathbf{D} + N_s(\mathbf{A}\mathbf{D} + \mathbf{D}\mathbf{A})] : \mathbf{D} \leq 0. \end{aligned} \quad (3.6)$$

Since (3.6) must hold for all incompressible flows, we may replace \mathbf{L} by $\alpha\mathbf{L}$, where α is any real number: this gives the inequality

$$\alpha[K - (\text{sgn } \alpha)B] - \alpha^2 C \leq 0, \quad (3.7)$$

in which

$$\rho^{-1}K = \Psi_{\mathbf{F}} \mathbf{F}^{\text{T}} : \mathbf{L} + \Psi_{\mathbf{A}} : [\mathbf{A}\mathbf{W} - \mathbf{W}\mathbf{A} + \lambda(\mathbf{A}\mathbf{D} + \mathbf{D}\mathbf{A} - 2\mathbf{A}\mathbf{D})], \quad (3.8)$$

$$B = \rho C_1 |\mathbf{D}| \Psi_{\mathbf{A}} : (\mathbf{I} - n\mathbf{A}), \quad (3.9)$$

$$C = \mathbf{T}(\mathbf{D}, \mathbf{A}) : \mathbf{D} = 2\mu_1[\mathbf{D} + N_p\mathbf{A}\mathbf{D} + N_s(\mathbf{A}\mathbf{D} + \mathbf{D}\mathbf{A})] : \mathbf{D}. \quad (3.10)$$

Lemma 1. *Satisfaction of the reduced dissipation inequality for all incompressible flows consistent with the constitutive equations (2.27) and (2.28), together with the appropriate closure rules, implies that*

$$C \geq 0, \quad B \geq 0, \quad K \leq |B|. \quad (3.11)$$

Proof. Suppose first that $\alpha > 0$; then (3.7) can be written in the form

$$(K - B) - \alpha C \leq 0. \quad (3.12)$$

Since α can be chosen arbitrarily small, we must have

$$K - B \leq 0. \quad (3.13)$$

This in turn implies that

$$C \geq 0, \tag{3.14}$$

for otherwise it would be possible to choose α sufficiently large to violate the inequality (3.12).

Suppose next that $\alpha < 0$. Then (3.7) becomes

$$K + B + |\alpha|C \geq 0. \tag{3.15}$$

From this inequality we deduce that

$$K + B \geq 0, \quad \text{and} \quad C \geq 0. \tag{3.16}$$

The inequality (3.11)₁ now follows automatically from (3.14) and (3.16), while (3.11)₂ may be deduced from (3.13) and (3.16)₁. These two inequalities also yield (3.11)₃. \square

We see from (3.11), (3.8)–(3.10) that while (3.11)₂, and (3.11)₃ require a knowledge of the free energy function in order that they may be used to determine restrictions on the constitutive equations, (3.11)₁ provides a direct means of determining such restrictions, if any exist. We see also that it is only the constitutive equation for the stress that plays a role in the definition of C , so that the second law in the present context will provide a means of determining restrictions only on the stress, and not on the evolution equation (2.27) for \mathbf{A} .

From (3.10) and (3.11)₁ we obtain as the necessary condition, bearing in mind that $\mu_1 > 0$,

$$|\mathbf{D}|^2 + N_s(\mathbf{A}\mathbf{D} + \mathbf{D}\mathbf{A}) : \mathbf{D} + N_p\mathbf{A}\mathbf{D} : \mathbf{D} \geq 0. \tag{3.17}$$

The first term on the left-hand side is of course positive, as is the second term, for the following reasons. First, the coefficient of N_s is

$$(\mathbf{A}\mathbf{D} + \mathbf{D}\mathbf{A}) : \mathbf{D} = 2\mathbf{A} : \mathbf{D}^2,$$

from the symmetry of \mathbf{A} and of \mathbf{D} . Now if we express \mathbf{A} and \mathbf{D} in component form relative to the principal basis of \mathbf{A} , then

$$\mathbf{A} : \mathbf{D}^2 = \sum_{i=1}^n A_{ii} D_{ii}^2 \geq 0,$$

given the definition and properties of \mathbf{A} . We are thus left with the term $\mathbf{A}\mathbf{D} : \mathbf{D}$; any statement about the sign of this term will be related to the question as to whether the tensor \mathbf{A} is positive semi-definite; that is, we wish to know the conditions under which

$$\mathbf{A}\mathbf{D} : \mathbf{D} \geq 0 \tag{3.18}$$

for all symmetric \mathbf{D} which satisfy $\text{tr } \mathbf{D} = 0$. Further relevant information may be obtained by invoking the requirement of orthotropy exploited by Cintra and Tucker [3], and which should be satisfied by any closure rule; by arranging the components of \mathbf{D} in vector form according to

$$\mathbf{d} := [D_{11} \ D_{22} \ D_{33} \ 2D_{23} \ 2D_{13} \ 2D_{12}]^T,$$

we may write

$$\mathbf{A}\mathbf{D} : \mathbf{D} = \mathbf{d}^T \overline{\mathbf{A}} \mathbf{d}, \tag{3.19}$$

in which the matrix $\bar{\mathbf{A}}$ has the structure given in (2.15). The question of the positivity or otherwise of the expression in (3.18) now becomes one related to the eigenvalues of $\bar{\mathbf{A}}$; specifically, we require that the eigenvalues of this 6×6 matrix all be nonnegative. This in turn is equivalent to the requirement, from (2.15), that

$$\bar{A}_{ij} \geq 0 \quad \text{for } i, j = 1, 2, 3, j \neq i, \quad (3.20)$$

and if we denote by $\bar{\bar{\mathbf{A}}}$ the 3×3 matrix $(\bar{\bar{\mathbf{A}}})_{ij}$ ($i, j = 1, 2, 3$),

$$\text{that the eigenvalues of } \bar{\bar{\mathbf{A}}} \text{ be nonnegative.} \quad (3.21)$$

The requirement (3.20) is one that is easily checked for any given closure rule. The second requirement (3.21) can be rewritten as a lengthy and, in the present context, an unenlightening set of conditions on the components \bar{A}_{ij} . For example, a necessary and sufficient condition for positive semi-definiteness of $\bar{\bar{\mathbf{A}}}$ is that (a)

$$\bar{A}_{11} \geq 0;$$

(b)

$$\det \begin{pmatrix} \bar{A}_{11} & \bar{A}_{12} \\ \bar{A}_{21} & \bar{A}_{22} \end{pmatrix} \geq 0;$$

and (c)

$$\det \bar{\bar{\mathbf{A}}} \geq 0.$$

In the absence of a specific choice of closure rule, and hence of components \mathcal{A}_{ijkl} , these conditions provide no information about the positive-definiteness or otherwise of $\bar{\bar{\mathbf{A}}}$, and so it is not possible to draw any general conclusions about the compatibility of the stress equation with the second law of thermodynamics, even with the property that two of the three terms in (3.17) are nonnegative.

We now proceed to examine the condition $C \geq 0$ for the specific closures introduced in Section 2.

3.1. Linear closure

Substitution of (2.12) in (3.10) yields

$$7 \left(1 - \frac{2}{35} N_p \right) \mathbf{D} : \mathbf{D} + N(\mathbf{A}\mathbf{D} + \mathbf{D}\mathbf{A}) : \mathbf{D} \geq 0 \quad (3.22)$$

where

$$N = 2N_p + 7N_s.$$

The second term on the left-hand side of (3.22) is nonnegative, as we have seen earlier, and so we obtain

Theorem 1. *The constitutive equation (2.27) with the linear closure approximation (2.12) is compatible with the second law of thermodynamics if*

$$N_p \leq \frac{35}{2}. \quad (3.23)$$

It is worth observing here that the restriction (3.23) is one that was obtained also by Galdi and Reddy [9], who showed that the rest state is unstable, in the sense of Liapounov, for particle numbers exceeding the value of 35/2.

3.2. Quadratic closure

A repetition of the computations just carried out, this time using the closure rule (2.13), yields

$$|\mathbf{D}|^2 + N_p(\mathbf{A} : \mathbf{D})^2 + 2N_s\mathbf{A} : \mathbf{D}^2 \geq 0. \tag{3.24}$$

This inequality is valid for any flow field and orientation tensor field, and so the second law imposes no restrictions on the equation for the stress.

3.3. The Hinch–Leal (H&L1) closure

We return to (3.10) and consider the form taken by the term $\mathbf{AD} : \mathbf{D}$ for this closure. Upon substituting (3.14) in this expression, we find that

$$5\mathbf{AD} : \mathbf{D} = 6 \operatorname{tr}[(\mathbf{AD})^2] - (\mathbf{A} : \mathbf{D})^2. \tag{3.25}$$

The first term is of indeterminate sign, while the second term is negative, and thus it is not possible to determine restrictions for all possible flows.

It is useful, though, to consider the consequences of one particular flow, that of biaxial elongation, for which the evolution equation together with the H&L1 closure is known to give unphysical results [2]. This flow has the form

$$v_1 = \epsilon x_1, \quad v_2 = \epsilon x_2, \quad v_3 = -2\epsilon x_3 \tag{3.26}$$

relative to a set of cartesian coordinates, and the stretching is

$$\mathbf{D} = \epsilon \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}. \tag{3.27}$$

A straightforward, if somewhat tedious calculation reveals that, for this flow,

$$\operatorname{tr}(\mathbf{AD})^2 = \epsilon^2[(A_{11}^2 + 2A_{12}^2 + A_{22}^2) - 4(A_{13}^2 + A_{23}^2 - A_{33}^2)]. \tag{3.28}$$

Now for biaxial elongation flow, we have $A_{22} = A_{11} = A$, say, and so $A_{33} = 1 - 2A$ [2]. In addition, all off-diagonal components are zero. It follows from (3.25) and (3.28) that

$$5\mathbf{AD} : \mathbf{D} = 4\epsilon^2[18A^2 - 18A + 5], \tag{3.29}$$

which is easily shown to be nonnegative for $A \leq 1$. The remaining two terms in the expression for C are also nonnegative, and so we see that, while the evolution equation with the Hinch–Leal law leads to non-physical results for the case of biaxial elongation, as reported in [2], the constitutive equation for the stress is consistent with the second law.

3.4. The smooth orthotropic closure rule

We turn now to the rule defined by (2.18) and (2.19), and substitute these values in (3.10). We consider the term $\mathbf{AD} : \mathbf{D}$ in the form (3.19), and in particular investigate the requirement (3.21). Now $\overline{\mathbf{A}}$ may be written in the form

$$\overline{\mathbf{A}} = \Gamma_0 + \Gamma_1 A_1 + \Gamma_2 A_2, \quad (3.30)$$

in which, from (2.18) and (2.19)

$$\Gamma_0 = \begin{pmatrix} -0.15 & 0.05 & 0.20 \\ 0.05 & -0.15 & 0.20 \\ 0.20 & 0.20 & 0.60 \end{pmatrix}, \quad \Gamma_1 = \begin{pmatrix} 1.15 & 0.05 & -0.20 \\ 0.05 & 0.15 & -0.20 \\ -0.20 & -0.20 & 0.60 \end{pmatrix},$$

and

$$\Gamma_2 = \begin{pmatrix} -0.10 & 0.30 & -0.20 \\ 0.30 & 0.90 & -0.20 \\ 0.30 & -0.20 & -0.60 \end{pmatrix}.$$

Thus, in order that C be nonnegative for all values of A_1 and A_2 in their ranges of physical validity, each of the matrices Γ_i ($i = 0, 1, 2$) must be positive semi-definite. In other words, the second law implies, under these general conditions, that all of the eigenvalues of the matrices Γ_i are nonnegative.

A routine calculation reveals, however, that the sets λ_i of eigenvalues of Γ_i are given by

$$\lambda_0 = [-0.2 \quad 0.2 \quad 0.7], \quad \lambda_1 = [0.19 \quad 1.18 \quad -0.67], \quad \lambda_2 = [-0.14 \quad -0.68 \quad 1.02],$$

which contradicts the necessary condition. Thus, while there may well exist admissible flows for which the smooth orthotropic closure is consistent with the second law, it cannot be said to be consistent for all such flows.

3.5. The natural closure

We use the closure defined by (2.20) and (2.21), and first note, using (2.22) and the incompressibility condition, that

$$\mathbf{AD} : \mathbf{D} = \frac{1}{3}[(\mathbf{A} : \mathbf{D})^2 + 2 \operatorname{tr}[(\mathbf{AD})^2]] + \frac{\Delta}{3}|\mathbf{D}|^2. \quad (3.31)$$

It follows that

$$C = \mathbf{T} : \mathbf{D} = 2\mu_1 \left(\frac{1}{3}N_p(\mathbf{A} : \mathbf{D})^2 + \frac{2}{3}N_p \operatorname{tr}[(\mathbf{AD})^2] + \left(1 + \frac{N_p\Delta}{3}\right)|\mathbf{D}|^2 + 2N_s\mathbf{A} : \mathbf{D}^2 \right). \quad (3.32)$$

The first, third and last terms on the right-hand side are clearly nonnegative (note that $\Delta \geq 0$, since the determinant is simply the product of the eigenvalues of \mathbf{A} , and these are nonnegative). To see that the term $\operatorname{tr}[(\mathbf{AD})^2]$ is nonnegative we expand it relative to the principal basis of \mathbf{A} , for which case

$$\mathbf{A} = \begin{pmatrix} A_{11} & 0 \\ 0 & A_{22} \end{pmatrix},$$

and find that

$$\text{tr}[(\mathbf{AD})^2] = (A_{11}D_{11})^2 + (A_{22}D_{22})^2 + 2A_{11}A_{22}D_{12}^2$$

which is of course nonnegative.

Thus the two-dimensional natural closure is consistent with the second law of thermodynamics.

4. Energetic stability

We begin by establishing an identity involving the kinetic energy of the fluid. We take the scalar product of (2.25) with \mathbf{v} , integrate over Ω and integrate by parts, to obtain

$$\frac{1}{2} \frac{d}{dt} \int_{\Omega} \rho |\mathbf{v}|^2 dx + \int_{\Omega} \mathbf{T} : \mathbf{L} dx = \int_{\Gamma} \mathbf{v} \cdot \mathbf{Tn} da + \int_{\Omega} \rho \mathbf{v} \cdot \mathbf{b} dx \tag{4.1}$$

where \mathbf{n} is the unit outward normal vector to Γ . We assume that the body is mechanically isolated [5], so that

$$\int_{\Gamma} \mathbf{v} \cdot \mathbf{Tn} da + \int_{\Omega} \rho \mathbf{v} \cdot \mathbf{b} dx = 0. \tag{4.2}$$

The kinetic energy E of the fluid is defined by

$$E(t) = \frac{1}{2} \int_{\Omega} \rho |\mathbf{v}|^2 dx,$$

and so we have, using (3.10),

$$E'(t) = - \int_{\Omega} \mathbf{T} : \mathbf{L} dx = - \int_{\Omega} C dx. \tag{4.3}$$

We will be interested first in determining the conditions under which fibre suspension flows are monotonically stable, for various closure approximations, in the sense that

$$E'(t) \leq 0 \quad \text{for all } t. \tag{4.4}$$

The energetic stability of the suspension, which is a global condition, is seen from (4.3) to be intimately connected to the local thermodynamic consistency condition $C \geq 0$.

Substitution of (2.27) in (4.3) and use of the incompressibility condition leads to the expression

$$E'(t) = -2\mu_1 \|\mathbf{D}\|^2 - 2\mu_1 \int_{\Omega} (2N_s \mathbf{A} : \mathbf{D}^2 + N_p \mathbf{AD} : \mathbf{D}) dx; \tag{4.5}$$

here and henceforth we use the notation

$$\|\mathbf{D}\| = \left[\int_{\Omega} \mathbf{D} : \mathbf{D} dx \right]^{1/2}$$

to denote the L^2 norm.

4.1. The linear closure approximation

Substitution of (2.12) in (4.5) leads to the expression

$$E'(t) = -\frac{4\mu_1 N}{7} \int_{\Omega} \mathbf{A} : \mathbf{D}^2 \, dx - 2\mu_1 \left(1 - \frac{2}{35} N_p\right) \|\mathbf{D}\|^2 \quad (4.6)$$

for the rate of change of kinetic energy. For all $t > 0$, and for all admissible fields \mathbf{v} and \mathbf{A} , we see from (4.6) and from the positivity of $\mathbf{A} : \mathbf{D}^2$ that (4.4) holds in the event that $N_p \leq 35/2$. Thus approximations with the linear closure are monotonically stable if $N_p \leq 35/2$.

We can go one step further, by recalling that, from Korn's inequality and the Poincaré–Friedrichs inequality (see, for example, [11]) there exists a constant $c_1 > 0$ such that

$$\|\mathbf{D}\|^2 \geq c_1 E(t); \quad (4.7)$$

thus, from (4.6) we have

$$E'(t) + \lambda E(t) \leq E'(t) + 2/\mu_1 \left(1 - \frac{2}{35} N_p\right) \|\mathbf{D}\|^2 = -\frac{4}{7} \times \frac{2C_1}{\mu_1} N \int_{\Omega} \mathbf{A} : \mathbf{D}^2 \, dx \leq 0, \quad (4.8)$$

where

$$\lambda = \frac{2c_1\mu_1}{\rho} \left(1 - \frac{2N_p}{35}\right).$$

It follows, by integration of (4.8), that

$$E(t) \leq E(0)e^{-\lambda t} \quad (4.9)$$

for all t . In other words, flows approximated by the linear closure are exponentially stable if $N_p \leq 35/2$.

4.2. The quadratic closure

For this closure, (4.5) takes the form

$$E'(t) + 2\mu_1 \|\mathbf{D}\|^2 = -2\mu_1 \left(N_p \int_{\Omega} (\mathbf{A} : \mathbf{D})^2 \, dx + 2N_s \int_{\Omega} \mathbf{A} : \mathbf{D}^2 \, dx \right) \leq 0. \quad (4.10)$$

We immediately deduce the monotonic stability from (4.10), and by application of the inequalities of Korn and Poincaré–Friedrichs as before, find that flows are in addition exponentially stable.

For the Hinch–Leal and smooth orthotropic closure rules, the sign-indeterminacy of $\mathbf{A} \mathbf{D} : \mathbf{D}$ in (4.5) does not permit any conclusions to be drawn about the stability, or otherwise, of flows approximated by these closures.

For the natural closure, an argument identical to that used in the case of the quadratic closure yields the result that two-dimensional flows are exponentially stable. We summarise the results for the linear, quadratic and natural closures in the following theorem.

Theorem 2. (a) *If $N_p \leq 35/2$, then fibre suspension flows corresponding to the linear closure approximation are monotonically stable, in the sense that*

$$E'(t) \leq 0. \quad (4.11)$$

Furthermore, such flows are exponentially stable, in the sense that there exists a positive constant λ such that

$$E(t) \leq E(0)e^{-\lambda t} \quad (4.12)$$

for all t .

(b) Fibre suspension flows corresponding to the quadratic closure approximation are monotonically and exponentially stable.

(c) Two-dimensional fibre suspension flows corresponding to the natural closure are monotonically and exponentially stable.

5. Conclusions

This study has focussed on the influence of the choice of closure rule on thermodynamic compatibility, and on energetic stability. With regard to the former, the second law, in the form of a dissipation inequality, has been used as a means of determining the restrictions, if any, which must be met by the constitutive equations. In the present context it is restrictions on the constitutive equation for the stress that are relevant.

The study has not been exhaustive, in the sense that only a selection of closure rules has been chosen for investigation. Nevertheless, each of the closures studied performs well in selected flow situations, and the spectrum of flows which is modelled accurately by at least one of the closures in the study is quite comprehensive.

The techniques and results presented here provide an additional means of assessing the degree of acceptability of closure rules, over and above existing rheological or numerical assessments. Indeed, the second law of thermodynamics places a simple restriction on the choice of particle number as a requirement for consistency, in the case of the linear closure; on the other hand, the results in respect of the Hinch–Leal closure are inconclusive, while the smooth orthotropic closure is shown, despite its good performance in selected flow simulations, not to be consistent for all possible flows. The quadratic and natural closures are consistent, the latter at least in the two-dimensional case.

Other closure rules may also be investigated using the methods presented here; the extent to which it is possible to obtain simple restrictions on such closures, for example in the form of bounds on material constants, will depend on the degree of complexity of the closures.

This study has provided no information on the properties of the evolution equation for the orientation tensor; such a complementary investigation would contribute towards a more complete understanding of the role of closure approximations.

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