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On a variational principle for the Upper Convected Maxwell model

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ABSTRACT

A variational principle for the Upper Convected Maxwell model is presented. The stationary value of the appropriate functional is the drag on an immersed object. From the principle, a formula is derived for the derivative of the drag with respect to the Deborah number for an arbitrarily shaped particle in a circular duct under creeping flow conditions. The formalism is compared with the conventional reciprocal theorem. Whereas the reciprocal theorem gives the drag as a volume integral involving the Stokesian stress tensor, the variational principle involves the stress from the adjoint equation. For low Deborah numbers both approaches provide the correction to the Stokes drag as a volume integral involving only the Stokesian rate-of-strain tensor, in line with second-order fluid theory.

1. Introduction

One of the classical variational principles in fluid mechanics is a principle due to Helmholtz [1]. It states that the motion of an incompressible Newtonian fluid at steady-state creeping flow conditions is characterized by minimum dissipation. That is, the dissipation is less than in any other motion that has the same velocity on the bounding surface of the flow domain. Extensions of the principle to non-Newtonian fluids and reformulations have been made by various authors [2–8] (see also [9], Chapter 8). Pawlowski [2] and, independently, Bird [3,4] extended the principle to the generalized Newtonian fluid, where the viscosity may be a function of the invariants of the rate-of-strain tensor. As Bird [3] observes, in general the flow does not minimize the dissipation, except for the relatively simple power law (Ostwald–de Waele) fluid. For this fluid Tomita [5] formulated the appropriate principle and applied it to estimate the drag on a sphere in an unbounded domain as a function of the power law index by inserting appropriate trial fields into the variational functional. Johnson [6] further developed the principle by extending it to fluids where the stress is obtained as the derivative of a function with respect to the strain rate. Also, the variational scheme encompasses cases where part of the bounding surface has force rather than velocity boundary conditions. Furthermore, alternative formulations leading to a maximum principle rather than a minimum principle are provided. Using these, Slattery [10] and Slattery and Wasserman [11] obtained upper and lower bounds for the drag on a sphere in a power law fluid. Schechter [7] reformulated the principle to calculate the flow pattern of power law fluids in ducts by minimizing the appropriate functional involving an imposed pressure gradient. More examples of flow profile estimates are given in ([8], Section 4.3). Tripathi and Chhabra [12]

found bounds for the drag in a bank of cylinders using the Carreau viscosity equation [8].

The various forms of the principle mentioned above have in common that the relation between stress and strain rate is essentially algebraic, whereby differential constitutive models such as the Upper Convected Maxwell model or Oldroyd-B model [8,13,14] are excluded. It is the purpose of this paper to explore a variational principle for the Upper Convected Maxwell (UCM) model with a meaningful physical quantity as its stationary value, namely the drag on an immersed particle. Specifically, using the principle we study the drag on an arbitrarily shaped particle in a circular duct (Fig. 1), where the rheology of the fluid is described by the UCM model and the flow condition is creeping flow. The particle is considered immobile, the flow steady and the flow speed far upstream (at inlet I), far downstream (at outlet O) and at the wall W of the duct is assumed to have a specified constant value U . On the particle P a stick boundary condition is imposed. By switching to a reference frame where the flow speed at I , O and W is zero, we see that these conditions may for example describe the slow settling of a particle under the influence of gravity in a vertical duct filled with stagnant fluid, with stick boundary conditions on W and with the proviso that the motion is considered purely translational. For the special case of a sphere on the axis of the duct, this is a standard geometry and a well-known test case for numerical studies at high Deborah numbers (see e.g. [15–18]).

Apart from presenting the variational scheme, we will also elaborate on the so-called reciprocal theorem and discuss the similarities and differences with the variational method. The comparison is justified by the status of the reciprocal theorem as a classic expedient in a multitude

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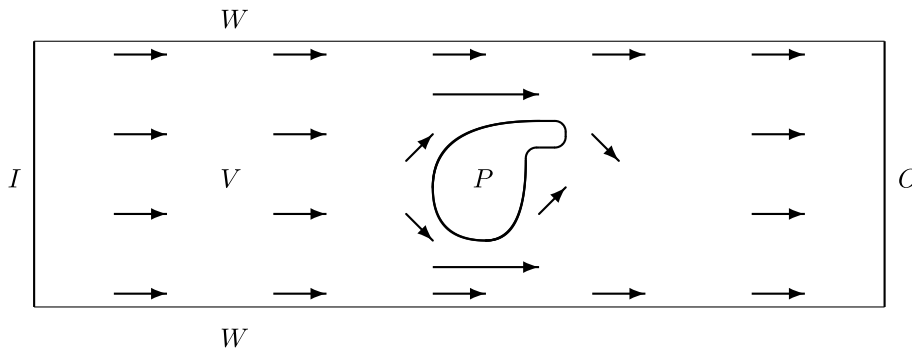


Fig. 1. Sectional view of a particle P in a circular duct. The wall, inlet and outlet are indicated with W , I and O , respectively. Also, V indicates the flow domain.

of studies of integral properties of flows and transport processes (for an accessible and comprehensive review see [19]). In the context of non-Newtonian fluids and creeping flow conditions, the theorem has found use in a number of studies focusing on the force and torque on particles at low Deborah number, where the theory of second-order fluids applies and one is especially interested in the corrections to the results obtained for Newtonian fluids. Well-known early studies include the work by Leal on the motion of slender particles [20] and by Brunn investigating the dynamics of particles of more general shape [21]. As emphasized in [19], it is one of the attractive features of the theorem that the corrections may be found directly in terms of parameters relating to Stokes flow, whereby the need to actually solve the relevant equations for the flow variables is circumvented. Chilcott and Rallison [22] employed the theorem to find an expression for the drag convenient for numerical computation in their work on creeping polymer flow around spheres and cylinders at arbitrary Deborah numbers. Extended versions of the reciprocal theorem incorporating both inertial and viscoelastic effects were used by Becker et al. [23] in their study on the sedimentation of a sphere near a plane wall, and by Dabade et al. [24] in their work on settling of anisotropic particles. A related use of the reciprocal theorem is in studies of self-propulsion in non-Newtonian fluids at small length scales, see e.g. [25–31]. A recent application is the investigation of flow rate-pressure drop relationships for complex fluids in narrow non-uniform geometries [32,33]. We will discuss the reciprocal theorem in the context of the variational study as described above.

The paper is organized as follows. After an introduction to the governing equations in Section 2, in Section 3 we present a variational principle for the UCM model. Among the conditions of stationarity of the variational functional are the equation of continuity, the equation of motion and the equation for the stress pertaining to the UCM model. Moreover, the stationary value of the functional is the drag on the particle. A direct consequence of the principle is a formula for the derivative of the drag with respect to Deborah number. In Section 4 we contrast this with the drag formula from the reciprocal theorem. It is remarked that both the variational principle and the reciprocal theorem do not rely on the Deborah number being small. However, their most obvious and simple use is at low Deborah numbers. In correspondence with second-order fluid theory the first-order correction in Deborah number is found as an integral involving the Stokesian rate-of-strain tensor. This is discussed in Section 5, where some immediate consequences of the correction are also outlined. Section 6 deals with the incorporation of other rheological models than the UCM model into the variational framework. We also establish a formal connection between the present variational scheme and the Pawlowski–Bird functional for the generalized Newtonian fluid ([3], Eqs. (12)–(15)). Finally, concluding remarks are presented in Section 7.

2. Governing equations

In this section we formulate the equations pertaining to the UCM problem. We prefer to use non-dimensionalized quantities as follows.

The position vector \mathbf{r} (directed from a suitably defined origin) and the flow velocity \mathbf{v} are non-dimensionalized with a characteristic size l of the particle and the main stream speed U , respectively. The viscosity η , which is a constant in the UCM model, is non-dimensionalized with a suitably chosen reference viscosity η_r , and the pressure p and stress tensor $\boldsymbol{\tau}$ with $\eta_r U/l$. Finally, the UCM relaxation time λ (see e.g. [14]) is non-dimensionalized with l/U . Explicitly,

$$\tilde{\mathbf{v}} = \mathbf{v}/U, \quad \tilde{\mathbf{r}} = \mathbf{r}/l, \quad (1)$$

$$\tilde{\eta} = \eta/\eta_r, \quad \tilde{p} = \frac{p l}{\eta_r U}, \quad \tilde{\boldsymbol{\tau}} = \frac{\boldsymbol{\tau} l}{\eta_r U}, \quad (2)$$

$$\tilde{\lambda} = \lambda U/l, \quad (3)$$

where the tilde indicates the non-dimensional quantities. It is noted that $\tilde{\lambda}$ serves as the dimensionless Deborah number. From now on we work exclusively with non-dimensionalized quantities and omit the tildes.

On the inlet I and outlet O (Fig. 1) the flow velocity \mathbf{v} equals the unit vector $\hat{\mathbf{U}}$ directed along the axis of the duct. It is convenient to also use

$$\mathbf{u}(\mathbf{r}) = \mathbf{v}(\mathbf{r}) - \hat{\mathbf{U}}, \quad (4)$$

where \mathbf{u} is the deviation of the flow velocity from the constant vector $\hat{\mathbf{U}}$.

Under the assumption of incompressibility of the fluid, the equation of continuity reads

$$\nabla \cdot \mathbf{u}(\mathbf{r}) = 0. \quad (5)$$

Under steady-state and creeping flow conditions, where inertia may be neglected, the equation of motion is

$$\mathbf{0} = -\nabla p(\mathbf{r}) + \nabla \cdot \boldsymbol{\tau}(\mathbf{r}), \quad (6)$$

where the stress tensor $\boldsymbol{\tau}$ is symmetric. Under steady-state conditions, in the UCM model $\boldsymbol{\tau}$ satisfies the equation (see e.g. [14])

$$\lambda(\mathbf{v} \cdot \nabla \boldsymbol{\tau} - \boldsymbol{\tau} \cdot \mathbf{L}^\dagger - \mathbf{L} \cdot \boldsymbol{\tau}) + \boldsymbol{\tau} = 2\eta \mathbf{d}, \quad (7)$$

where \mathbf{L} denotes the velocity gradient tensor $(\nabla \mathbf{v})^\dagger$ (\dagger denoting a transposition). Also, we have

$$\mathbf{d} = \frac{1}{2}(\mathbf{L} + \mathbf{L}^\dagger), \quad (8)$$

the rate-of-strain tensor. For $\lambda = 0$ we have Stokes flow.

As for the boundary conditions, on the inlet I and outlet O (Fig. 1) the fluid flows without UCM stress with velocity $\mathbf{v} = \hat{\mathbf{U}}$, so we have

$$\mathbf{u}(\mathbf{r}) = \mathbf{0}, \quad \boldsymbol{\tau}(\mathbf{r}) = \mathbf{0} \quad \text{on } I, O. \quad (9)$$

On the wall W of the duct the fluid flows with velocity $\hat{\mathbf{U}}$, so

$$\mathbf{u}(\mathbf{r}) = \mathbf{0} \quad \text{on } W. \quad (10)$$

Finally, we have

$$\mathbf{u}(\mathbf{r}) = -\hat{\mathbf{U}} \quad \text{on } P, \quad (11)$$

since we assume the flow velocity \mathbf{v} to be zero on the particle.

The force \mathbf{F} on the particle is given by

$$\mathbf{F} = \int_P dS \mathbf{n} \cdot (p \boldsymbol{\delta} - \boldsymbol{\tau}) \quad (12)$$

where dS denotes an element of surface, $\boldsymbol{\delta}$ is the Kronecker delta and \mathbf{n} is the unit normal on the surface pointing outside V . From \mathbf{F} we obtain

$$D = \hat{\mathbf{U}} \cdot \mathbf{F} \quad (13)$$

as the drag D on the particle.

3. A variational principle for the UCM model

We wish to formulate a functional where the conditions of stationarity with respect to variations of the trial fields include the relevant equations from Section 2. Also, at these conditions we require the functional to be equal to the drag on the particle. The question arises how one can construct such a functional. First of all, it is clear by inspection of the principles outlined in the Introduction that the pressure is a Lagrange multiplier for the condition that the divergence of the velocity field be zero. Also, the variation of the velocity should produce the equation of motion (6). It is logical to suppose that in the case of the UCM model the variation of the stress tensor should generate the stress Eq. (7).

It is here that we encounter a difference with the principles mentioned before. In contrast with the generalized Newtonian fluid, in the UCM model the stress Eq. (7) is so complex that building a satisfactory functional from $(p, \mathbf{u}, \boldsymbol{\tau})$ seems impossible. However, proceeding in the spirit of ([9], Chapters 8–10) we may consider an extension of the functional whereby the set of trial functions is enlarged to a set $(p_1, \mathbf{u}_1, \boldsymbol{\tau}_1, p_2, \mathbf{u}_2, \boldsymbol{\tau}_2)$ such that the variations of $(p_1, \mathbf{u}_1, \boldsymbol{\tau}_1)$ lead to Eqs. (5)–(7) for $(p_2, \mathbf{u}_2, \boldsymbol{\tau}_2)$. The equations for $(p_1, \mathbf{u}_1, \boldsymbol{\tau}_1)$ resulting from variations of $(p_2, \mathbf{u}_2, \boldsymbol{\tau}_2)$ (the ‘adjoint’ equations) are similar to but not necessarily identical to Eqs. (5)–(7). Importantly, the stationary value of the extended functional must be the drag relating to the fields $(p_2, \mathbf{u}_2, \boldsymbol{\tau}_2)$.

Consider the functional

$$\begin{aligned} X = & \int_V dV (p_1 \nabla \cdot \mathbf{u}_2 - \mathbf{u}_1 \cdot \nabla p_2) \\ & + \int_V dV \frac{\lambda}{2\eta} \boldsymbol{\tau}_1 : (\mathbf{v}_2 \cdot \nabla \boldsymbol{\tau}_2 - \boldsymbol{\tau}_2 \cdot \mathbf{L}_2^\dagger - \mathbf{L}_2 \cdot \boldsymbol{\tau}_2) \\ & + \int_V dV \left(\frac{1}{2\eta} \boldsymbol{\tau}_1 : \boldsymbol{\tau}_2 - \boldsymbol{\tau}_1 : \mathbf{d}_2 + \mathbf{u}_1 \cdot (\nabla \cdot \boldsymbol{\tau}_2) \right) \\ & + \int_P dS \hat{\mathbf{U}} \cdot (\mathbf{n} \cdot (p_2 \boldsymbol{\delta} - \boldsymbol{\tau}_2)), \end{aligned} \quad (14)$$

where the fields \mathbf{v}_2 , \mathbf{L}_2 and \mathbf{d}_2 relate to \mathbf{u}_2 in line with the formulae from Section 2,

$$\mathbf{v}_2(\mathbf{r}) = \hat{\mathbf{U}} + \mathbf{u}_2(\mathbf{r}), \quad \mathbf{L}_2(\mathbf{r}) = (\nabla \mathbf{v}_2)^\dagger, \quad \mathbf{d}_2(\mathbf{r}) = \frac{1}{2}(\mathbf{L}_2 + \mathbf{L}_2^\dagger). \quad (15)$$

We impose that $\boldsymbol{\tau}_1$ and $\boldsymbol{\tau}_2$ are symmetric (like $\boldsymbol{\tau}$), and furthermore

$$\mathbf{u}_1(\mathbf{r}) = \mathbf{u}_2(\mathbf{r}) = \mathbf{0}, \quad \boldsymbol{\tau}_1(\mathbf{r}) = \boldsymbol{\tau}_2(\mathbf{r}) = \mathbf{0} \quad \text{on } I, O, \quad (16)$$

$$\mathbf{u}_1(\mathbf{r}) = \mathbf{u}_2(\mathbf{r}) = \mathbf{0} \quad \text{on } W, \quad (17)$$

$$\mathbf{u}_1(\mathbf{r}) = +\hat{\mathbf{U}}, \quad \mathbf{u}_2(\mathbf{r}) = -\hat{\mathbf{U}} \quad \text{on } P. \quad (18)$$

These conditions correspond to (9)–(11), except for a reversed flow condition for \mathbf{u}_1 . Indeed, \mathbf{u}_1 indicates a deviation of the flow velocity \mathbf{v}_1 from $-\hat{\mathbf{U}}$,

$$\mathbf{v}_1(\mathbf{r}) = -\hat{\mathbf{U}} + \mathbf{u}_1(\mathbf{r}), \quad (19)$$

$$\mathbf{v}_1(\mathbf{r}) = -\hat{\mathbf{U}} \quad \text{on } I, O, W, \quad (20)$$

$$\mathbf{v}_1(\mathbf{r}) = \mathbf{0} \quad \text{on } P, \quad (21)$$

corresponding to a reversed flow in the duct.

Next we find the conditions for stationarity of the functional with respect to variations of the trial fields. With the help of the divergence theorem the first variation of X is found as

$$\begin{aligned} \delta X = & \int_V dV (\delta p_1 \nabla \cdot \mathbf{u}_2 + \delta \mathbf{u}_1 \cdot (-\nabla p_2 + \nabla \cdot \boldsymbol{\tau}_2)) \\ & + \int_V dV \delta \boldsymbol{\tau}_1 : \frac{\lambda}{2\eta} (\mathbf{v}_2 \cdot \nabla \boldsymbol{\tau}_2 - \boldsymbol{\tau}_2 \cdot \mathbf{L}_2^\dagger - \mathbf{L}_2 \cdot \boldsymbol{\tau}_2) \\ & + \int_V dV \delta \boldsymbol{\tau}_1 : \frac{1}{2\eta} (\boldsymbol{\tau}_2 - 2\eta \mathbf{d}_2) \\ & + \int_V dV (\delta p_2 \nabla \cdot \mathbf{u}_1 + \delta \mathbf{u}_2 \cdot (-\nabla p_1 + \lambda \mathbf{c} + \nabla \cdot \boldsymbol{\tau}_1)) \\ & + \int_V dV \delta \boldsymbol{\tau}_2 : \frac{\lambda}{2\eta} (-\nabla \cdot (\mathbf{v}_2 \boldsymbol{\tau}_1) - \mathbf{L}_2^\dagger \cdot \boldsymbol{\tau}_1 - \boldsymbol{\tau}_1 \cdot \mathbf{L}_2) \\ & + \int_V dV \delta \boldsymbol{\tau}_2 : \frac{1}{2\eta} (\boldsymbol{\tau}_1 - 2\eta \mathbf{d}_1) \\ & + \int_S dS \mathbf{n} \cdot (-\delta p_2 \mathbf{u}_1 - \frac{\lambda}{\eta} \delta \mathbf{u}_2 \cdot \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 - \delta \mathbf{u}_2 \cdot \boldsymbol{\tau}_1) \\ & + \int_S dS \mathbf{n} \cdot \left(\frac{\lambda}{2\eta} \mathbf{v}_2 \delta \boldsymbol{\tau}_2 : \boldsymbol{\tau}_1 + \delta \boldsymbol{\tau}_2 \cdot \mathbf{u}_1 \right) \\ & + \int_P dS \hat{\mathbf{U}} \cdot (\mathbf{n} \cdot (\delta p_2 \boldsymbol{\delta} - \delta \boldsymbol{\tau}_2)) \end{aligned} \quad (22)$$

with \mathbf{c} and \mathbf{d}_1 given by

$$\mathbf{c} = \frac{1}{2\eta} ((\nabla \boldsymbol{\tau}_2) : \boldsymbol{\tau}_1 + 2\nabla \cdot (\boldsymbol{\tau}_2 \cdot \boldsymbol{\tau}_1)), \quad (23)$$

$$\mathbf{L}_1(\mathbf{r}) = (\nabla \mathbf{v}_1)^\dagger, \quad \mathbf{d}_1(\mathbf{r}) = \frac{1}{2}(\mathbf{L}_1 + \mathbf{L}_1^\dagger), \quad (24)$$

and S is a shorthand for $I + O + W + P$ (see Fig. 1).

We take into account the conditions (16)–(18) on the boundaries, where the corresponding variations of the fields are zero. On P four surface terms involving δp_2 and $\delta \boldsymbol{\tau}_2$ are seen to cancel by (18). The surface term with $\delta \boldsymbol{\tau}_2 : \boldsymbol{\tau}_1$ is zero on I and O because of (16), zero on W because $\mathbf{n} \cdot \hat{\mathbf{U}}$ is zero and because of (17), and zero on P because of (18). The remaining surface terms involve \mathbf{u}_1 , \mathbf{u}_2 or their variations and are zero as well. We are left with

$$\begin{aligned} \delta X = & \int_V dV (\delta p_1 \nabla \cdot \mathbf{u}_2 + \delta \mathbf{u}_1 \cdot (-\nabla p_2 + \nabla \cdot \boldsymbol{\tau}_2)) \\ & + \int_V dV \delta \boldsymbol{\tau}_1 : \frac{\lambda}{2\eta} (\mathbf{v}_2 \cdot \nabla \boldsymbol{\tau}_2 - \boldsymbol{\tau}_2 \cdot \mathbf{L}_2^\dagger - \mathbf{L}_2 \cdot \boldsymbol{\tau}_2) \\ & + \int_V dV \delta \boldsymbol{\tau}_1 : \frac{1}{2\eta} (\boldsymbol{\tau}_2 - 2\eta \mathbf{d}_2) \\ & + \int_V dV (\delta p_2 \nabla \cdot \mathbf{u}_1 + \delta \mathbf{u}_2 \cdot (-\nabla p_1 + \lambda \mathbf{c} + \nabla \cdot \boldsymbol{\tau}_1)) \\ & + \int_V dV \delta \boldsymbol{\tau}_2 : \frac{\lambda}{2\eta} (-\nabla \cdot (\mathbf{v}_2 \boldsymbol{\tau}_1) - \mathbf{L}_2^\dagger \cdot \boldsymbol{\tau}_1 - \boldsymbol{\tau}_1 \cdot \mathbf{L}_2) \\ & + \int_V dV \delta \boldsymbol{\tau}_2 : \frac{1}{2\eta} (\boldsymbol{\tau}_1 - 2\eta \mathbf{d}_1) \end{aligned} \quad (25)$$

as the first variation.

As a consequence, from the requirement of stationarity of X we obtain the following equations. As for the fields with label 2, \mathbf{u}_2 satisfies the equation of continuity (5) and the equation of motion (6). The stress tensor $\boldsymbol{\tau}_2$ satisfies (7). So we may identify

$$\mathbf{u}_2 = \mathbf{u}, \quad p_2 = p, \quad \boldsymbol{\tau}_2 = \boldsymbol{\tau}. \quad (26)$$

The fields with label 1 satisfy adjoint equations closely related to the equations found for label 2. The velocity field \mathbf{u}_1 satisfies (5) and an equation of motion

$$-\nabla p_1 + \lambda \mathbf{c} + \nabla \cdot \boldsymbol{\tau}_1 = \mathbf{0} \quad (27)$$

which is (6) apart from the additional $\lambda \mathbf{c}$. The equation for the stress tensor $\boldsymbol{\tau}_1$ is found as

$$\lambda (-\mathbf{v}_2 \cdot \nabla \boldsymbol{\tau}_1 - \mathbf{L}_2^\dagger \cdot \boldsymbol{\tau}_1 - \boldsymbol{\tau}_1 \cdot \mathbf{L}_2) + \boldsymbol{\tau}_1 = 2\eta \mathbf{d}_1, \quad (28)$$

where we used the equation of continuity for \mathbf{u}_2 . We see that (28) has the structure of a Lower Convected Maxwell model for $\boldsymbol{\tau}_1$ [13], with the proviso that the convection and velocity gradient in the convective derivative correspond to $-\mathbf{v}_2$ rather than \mathbf{v}_1 .

Evaluation of X under the conditions of stationarity shows that the volume integrals in X are zero or cancel and we are left with

$$X^{stat} = \int_P dS \hat{\mathbf{U}} \cdot (\mathbf{n} \cdot (p_2 \boldsymbol{\delta} - \boldsymbol{\tau}_2)) = D. \tag{29}$$

Hence the drag may be obtained as the stationary value of the functional X .

The variational principle allows us to give a concise formula for the derivative of the drag with respect to the Deborah number. We consider the functional X for a certain value of λ and assume that the trial fields correspond to the conditions of stationarity. A change of λ generates two contributions to the change of the stationary value of X . The first contribution is due to the explicit dependence of X on λ . The second contribution comes from the change in the trial fields corresponding to the new stationary value of X . Because X is stationary under variations of the trial fields, we only need to take into account the first contribution and find

$$\frac{dX^{stat}}{d\lambda} = \frac{dD}{d\lambda} = \frac{1}{2\eta} \int_V dV \boldsymbol{\tau}_1 : (\mathbf{v}_2 \cdot \nabla \boldsymbol{\tau}_2 - \boldsymbol{\tau}_2 \cdot \mathbf{L}_2^\dagger - \mathbf{L}_2 \cdot \boldsymbol{\tau}_2) \tag{30}$$

by inspection of (14).

4. The reciprocal theorem

For the case under investigation, the reciprocal theorem may be derived as follows [19,22]. We write

$$\boldsymbol{\sigma} = -p\boldsymbol{\delta} + \boldsymbol{\tau} \tag{31}$$

and derive an expression for the difference between the drag D and the Stokes drag D_s (a subscript s denotes a Stokesian value). We have

$$\begin{aligned} D - D_s &= \hat{\mathbf{U}} \cdot (\mathbf{F} - \mathbf{F}_s) \\ &= \int_P dS \mathbf{n} \cdot (-\boldsymbol{\sigma} + \boldsymbol{\sigma}_s) \cdot \hat{\mathbf{U}} \\ &= \int_S dS \mathbf{n} \cdot (\boldsymbol{\sigma} \cdot \mathbf{u}_s - \boldsymbol{\sigma}_s \cdot \mathbf{u}) \end{aligned} \tag{32}$$

where we used (9)–(11). Using the divergence theorem and the equation of motion (6) we obtain

$$\begin{aligned} D - D_s &= \int_V dV (\boldsymbol{\sigma} : \nabla \mathbf{u}_s - \boldsymbol{\sigma}_s : \nabla \mathbf{u}) \\ &= \int_V dV (\boldsymbol{\tau} : \nabla \mathbf{u}_s - \boldsymbol{\tau}_s : \nabla \mathbf{u}) \end{aligned} \tag{33}$$

where the last equality follows because the pressure contributions (see (31)) are zero due to (5). Finally, using (7) and (8) we find

$$\begin{aligned} D - D_s &= \int_V dV (\boldsymbol{\tau} : \mathbf{d}_s - \boldsymbol{\tau}_s : \mathbf{d}) \\ &= \frac{\lambda}{2\eta} \int_V dV \boldsymbol{\tau}_s : (-\mathbf{v} \cdot \nabla \boldsymbol{\tau} + \boldsymbol{\tau} \cdot \mathbf{L}^\dagger + \mathbf{L} \cdot \boldsymbol{\tau}) \end{aligned} \tag{34}$$

as the difference between the drag and the Stokes drag.

We may contrast the variational formula (30) and the reciprocal theorem (34) as follows,

$$\frac{dD}{d\lambda} = \frac{1}{2\eta} \int_V dV (-\boldsymbol{\tau}_1) : (-\mathbf{v} \cdot \nabla \boldsymbol{\tau} + \boldsymbol{\tau} \cdot \mathbf{L}^\dagger + \mathbf{L} \cdot \boldsymbol{\tau}), \text{ (var.)} \tag{35}$$

$$\frac{D - D_s}{\lambda} = \frac{1}{2\eta} \int_V dV \boldsymbol{\tau}_s : (-\mathbf{v} \cdot \nabla \boldsymbol{\tau} + \boldsymbol{\tau} \cdot \mathbf{L}^\dagger + \mathbf{L} \cdot \boldsymbol{\tau}). \text{ (rec.)} \tag{36}$$

In (35) the volume integral involves the adjoint stress tensor whereas (36) involves the Stokesian stress tensor.

5. The low Deborah number correction to the drag

A simple form of (30) can be derived for small λ . The flows reduce to Stokes flows,

$$-\mathbf{u}_1 = \mathbf{u}_2 = \mathbf{u}_s, \quad -\boldsymbol{\tau}_1 = \boldsymbol{\tau}_2 = \boldsymbol{\tau}_s, \tag{37}$$

$$\mathbf{v}_2 = \mathbf{v}_s = \hat{\mathbf{U}} + \mathbf{u}_s, \quad \mathbf{L}_2 = \mathbf{L}_s, \quad \mathbf{d}_2 = \mathbf{d}_s, \tag{38}$$

and we find

$$\left. \frac{dD}{d\lambda} \right|_{\lambda=0} = \frac{1}{2\eta} \int_V dV \boldsymbol{\tau}_s : (-\mathbf{v}_s \cdot \nabla \boldsymbol{\tau}_s + \boldsymbol{\tau}_s \cdot \mathbf{L}_s^\dagger + \mathbf{L}_s \cdot \boldsymbol{\tau}_s). \tag{39}$$

Using the divergence theorem and the boundary conditions on \mathbf{v}_s and $\boldsymbol{\tau}_s$ (cf. (16)–(18)) we may transform the first term (with $\mathbf{v}_s \cdot \nabla$) into its negative. As a consequence this term is zero so that, using $\boldsymbol{\tau}_s = 2\eta \mathbf{d}_s$ we obtain

$$\left. \frac{dD}{d\lambda} \right|_{\lambda=0} = 2\eta \int_V dV Tr \mathbf{d}_s^3, \tag{40}$$

Tr denoting the trace. Putting

$$D = D_s + \lambda D_c \tag{41}$$

where D_c indicates the correction to the drag to first order in the Deborah number, we find

$$D_c = 2\eta \int_V dV Tr \mathbf{d}_s^3 \tag{42}$$

as the correction in terms of Stokesian quantities.

It is directly seen from (36) that the reciprocal theorem leads to the same correction (42). The fact that the reciprocal theorem for a second-order fluid leads to drag formulae involving a volume integral over a product of Stokesian rate-of-strain tensors was already observed by Brunn [21,34]. For the present configuration, writing the stress tensor for a second-order fluid as

$$\boldsymbol{\tau} = 2\eta(\mathbf{d} + \alpha \mathring{\mathbf{d}} + \beta \mathbf{d} \cdot \mathbf{d}) \tag{43}$$

where $\mathring{\mathbf{d}}$ denotes the corotational deriviate [8] of \mathbf{d} , and proceeding as in Section 4, we have from the reciprocal theorem

$$D = D_s + (\alpha + \beta) D_c \quad \text{(second-order fluid, } \alpha, \beta \rightarrow 0) \tag{44}$$

with D_c from (42). The UCM formulae (41) and (42) are the special case $\alpha = -\lambda, \beta = 2\lambda$.

The correction (42) has as a consequence that for a number of configurations D_c will be zero. In Fig. 2 four configurations are given where a combination of time reversal and inversion (with respect to a suitable origin as indicated) produces the same or a physically similar configuration. In those cases

$$\mathbf{u}_s(\mathbf{r}) \xrightarrow{\text{time reversal}} -\mathbf{u}_s(\mathbf{r}) \xrightarrow{\text{inversion}} \mathbf{u}_s(-\mathbf{r}), \tag{45}$$

so that $\mathbf{d}_s(\mathbf{r}) = -\mathbf{d}_s(-\mathbf{r})$ and $D_c = 0$ follows. For the case of a sphere in an unbounded domain this result is already mentioned in the classic paper [35] concerning the second-order correction (see also [8]).

In Fig. 3 we have two cases where D_c will not be zero. This is essentially due to the fact that the fore-aft symmetry of the configuration is broken. The role of particle fore-aft symmetry in calculations of the force was already noted by Leal [20].

We have discussed the case of a particle in a duct. As is clear from the analysis, we may carry over the results to a two-dimensional (2D) setting. Here the duct is replaced by two parallel plates and the particle by a prismatic beam positioned perpendicular to the flow. The drag is considered per unit length of the beam. A direct consequence of (42) is then the following statement:

$$D_c = 0, \quad (2D) \tag{46}$$

stating that the first-order correction to the Stokes drag is zero. This is due to the fact that in 2D the incompressibility condition $Tr \mathbf{d}_s = 0$ implies $Tr \mathbf{d}_s^3 = 0$.

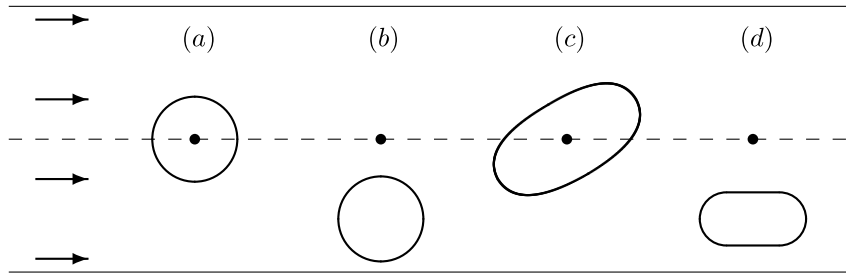


Fig. 2. Geometries with $D_c = 0$. (a) sphere on-axis, (b) sphere off-axis, (c) ellipsoid on-axis, non-aligned, (d) capsule off-axis, aligned with duct. The origins are indicated with \bullet .

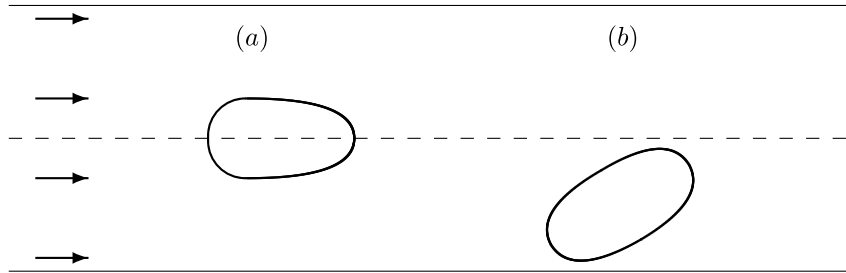


Fig. 3. Geometries with non-zero D_c . (a) egg-shaped particle, on-axis, aligned with duct, (b) ellipsoid off-axis, non-aligned.

We end this section with two observations. Firstly, it is remarked that if the Stokes flows (37) are inserted into the functional (14) by way of approximation of the actual flows, the variational approximation $X = D$ of the drag gives (41)–(42) without restriction on the Deborah number. Of course, the approximation will be very poor in general but does provide the first-order result. Secondly, the correction (42) may also be derived directly from the governing equations. We expand the fields to first order in λ as in (41), e.g.

$$\mathbf{u} = \mathbf{u}_s + \lambda \mathbf{u}_c \tag{47}$$

and similarly for p, τ , etc. We find from (5)–(7)

$$\nabla \cdot \mathbf{u}_s = 0 \quad , \quad \nabla \cdot \mathbf{u}_c = 0, \tag{48}$$

$$\mathbf{0} = -\nabla p_s + \nabla \cdot \boldsymbol{\tau}_s \quad , \quad \mathbf{0} = -\nabla p_c + \nabla \cdot \boldsymbol{\tau}_c, \tag{49}$$

$$\boldsymbol{\tau}_s = 2\eta \mathbf{d}_s, \tag{50}$$

$$\mathbf{v}_s \cdot \nabla \boldsymbol{\tau}_s - \boldsymbol{\tau}_s \cdot \mathbf{L}_s^\dagger - \mathbf{L}_s \cdot \boldsymbol{\tau}_s + \boldsymbol{\tau}_c = 2\eta \mathbf{d}_c. \tag{51}$$

The boundary conditions are

$$\mathbf{u}_s = \mathbf{0} \text{ on } I, O, W, \quad \mathbf{u}_s = -\hat{\mathbf{U}} \text{ on } P, \tag{52}$$

$$\mathbf{u}_c = \mathbf{0} \text{ on } I, O, W, P, \tag{53}$$

as seen from (9)–(11).

In the derivation we will make repeated use of the divergence theorem. From (51) we obtain

$$\frac{1}{2\eta} \int_V dV \boldsymbol{\tau}_s : (-\mathbf{v}_s \cdot \nabla \boldsymbol{\tau}_s + \boldsymbol{\tau}_s \cdot \mathbf{L}_s^\dagger + \mathbf{L}_s \cdot \boldsymbol{\tau}_s) = \frac{1}{2\eta} \int_V dV \boldsymbol{\tau}_s : (\boldsymbol{\tau}_c - 2\eta \mathbf{d}_c). \tag{54}$$

The term on the right with $\boldsymbol{\tau}_s : \mathbf{d}_c$ is found to vanish by (53), (48) and (49),

$$\begin{aligned} \int_V dV \boldsymbol{\tau}_s : \mathbf{d}_c &= \int_V dV \boldsymbol{\tau}_s : (\nabla \mathbf{u}_c) \\ &= \int_S dS \mathbf{n} \cdot (\mathbf{u}_c \cdot \boldsymbol{\tau}_s) - \int_V dV \mathbf{u}_c \cdot (\nabla \cdot \boldsymbol{\tau}_s) \\ &= - \int_V dV \mathbf{u}_c \cdot \nabla p_s \\ &= - \int_S dS \mathbf{n} \cdot \mathbf{u}_c p_s + \int_V dV (\nabla \cdot \mathbf{u}_c) p_s \\ &= 0. \end{aligned} \tag{55}$$

The remaining term on the right of (54) may be linked to the drag. We have

$$\begin{aligned} \frac{1}{2\eta} \int_V dV \boldsymbol{\tau}_s : \boldsymbol{\tau}_c &= \int_V dV \mathbf{d}_s : \boldsymbol{\tau}_c \\ &= \int_V dV (\nabla \mathbf{u}_s) : \boldsymbol{\tau}_c \\ &= \int_S dS \mathbf{n} \cdot (\mathbf{u}_s \cdot \boldsymbol{\tau}_c) - \int_V dV \mathbf{u}_s \cdot (\nabla \cdot \boldsymbol{\tau}_c) \\ &= - \int_P dS \mathbf{n} \cdot (\hat{\mathbf{U}} \cdot \boldsymbol{\tau}_c) - \int_V dV \mathbf{u}_s \cdot (\nabla \cdot \boldsymbol{\tau}_c) \end{aligned} \tag{56}$$

using (50) and (52). The first term on the right is the stress contribution to D_c , whereas the last term may be transformed into the pressure contribution,

$$\begin{aligned} - \int_V dV \mathbf{u}_s \cdot (\nabla \cdot \boldsymbol{\tau}_c) &= - \int_V dV \mathbf{u}_s \cdot \nabla p_c \\ &= - \int_S dS \mathbf{n} \cdot \mathbf{u}_s p_c + \int_V dV (\nabla \cdot \mathbf{u}_s) p_c \\ &= \int_P dS \mathbf{n} \cdot \hat{\mathbf{U}} p_c, \end{aligned} \tag{57}$$

where we used (49) and (48).

With (55)–(57) Eq. (54) becomes

$$\frac{1}{2\eta} \int_V dV \boldsymbol{\tau}_s : (-\mathbf{v}_s \cdot \nabla \boldsymbol{\tau}_s + \boldsymbol{\tau}_s \cdot \mathbf{L}_s^\dagger + \mathbf{L}_s \cdot \boldsymbol{\tau}_s) = \int_P dS \mathbf{n} \cdot (\hat{\mathbf{U}} p_c - \hat{\mathbf{U}} \cdot \boldsymbol{\tau}_c), \tag{58}$$

in correspondence with (39). Eq. (42) follows as before.

6. Other rheological models

In this section we discuss the possibility of incorporating other models than the UCM model into the variational framework. Also, we wish to establish a formal connection with the Pawlowksi–Bird principle for the generalized Newtonian fluid [2,3].

The UCM constitutive equation is only one of the many rheological models beyond the generalized Newtonian fluid [8,13], and the question arises how other models (for instance, the Oldroyd-B model or the Giesekus model) may be incorporated. Whatever the model is that we choose, we can formulate the relevant equations (continuity, motion, etc.) in the schematic form

$$0 = R H S(\mathbf{u}, \mathbf{d}, \boldsymbol{\tau}, \dots), \tag{59}$$

RHS meaning right hand side. With the logic of Section 3, all the fields in (59) get label 2. Schematically, the functional X is then formulated as

$$X = \int_V dV p_1 RHS(continuity)_2 \tag{60}$$

$$+ \int_V dV (\mathbf{u}_1 \cdot RHS(motion)_2 + \boldsymbol{\tau}_1 : RHS(stress)_2) + \dots$$

$$+ \int_P dS \hat{\mathbf{U}} \cdot (\mathbf{n} \cdot (p_2 \boldsymbol{\delta} - \boldsymbol{\tau}_2)).$$

This leads to the correct equations for the fields with label 2 and the stationary value of X is the drag, under the condition that the surface terms in δX disappear because of the boundary conditions (cf. (25)). This is best investigated on a case-by-case basis. For instance, we may consider a Giesekus-type extension of the UCM model,

$$\mathbf{0} = \lambda(\mathbf{v} \cdot \nabla \boldsymbol{\tau} - \boldsymbol{\tau} \cdot \mathbf{L}^\dagger - \mathbf{L} \cdot \boldsymbol{\tau}) + \boldsymbol{\tau} + \lambda \frac{\alpha}{\eta} \boldsymbol{\tau} \cdot \boldsymbol{\tau} - 2\eta \mathbf{d}, \tag{61}$$

with α a constant. The extra term X_{extra} to be added to (14) is

$$X_{extra} = \int_V dV \frac{1}{2\eta} \boldsymbol{\tau}_1 : (\lambda \frac{\alpha}{\eta} \boldsymbol{\tau}_2 \cdot \boldsymbol{\tau}_2), \tag{62}$$

and no extra surface terms are generated in the variation. The correct Eq. (61) is found for $\boldsymbol{\tau}_2$ at the expense of an extra term involving both $\boldsymbol{\tau}_1$ and $\boldsymbol{\tau}_2$ in the equation for $\boldsymbol{\tau}_1$. The stationary value of the extended functional is the drag resulting from (61).

To make the connection with the generalized Newtonian fluid, it is convenient to start from (14) and first reduce it to the Newtonian (constant viscosity) case (N). After that, we incorporate the generalized Newtonian (GN) model. We first put $\lambda = 0$ in (14), which gives

$$X_N = \int_V dV (p_1 \nabla \cdot \mathbf{u}_2 - \mathbf{u}_1 \cdot \nabla p_2)$$

$$+ \int_V dV (\frac{1}{2\eta} \boldsymbol{\tau}_1 : \boldsymbol{\tau}_2 - \boldsymbol{\tau}_1 : \mathbf{d}_2 + \mathbf{u}_1 \cdot (\nabla \cdot \boldsymbol{\tau}_2))$$

$$+ \int_P dS \hat{\mathbf{U}} \cdot (\mathbf{n} \cdot (p_2 \boldsymbol{\delta} - \boldsymbol{\tau}_2)). \tag{63}$$

Because the resulting equations for the fields with labels 1 and 2 are the same we can dispense with the labels. Also, using $\boldsymbol{\tau} = 2\eta \mathbf{d}$ we can leave out the variation of $\boldsymbol{\tau}$ and employ the smaller set (p, \mathbf{u}) . Explicitly, with reference to (37) we use

$$-p_1 = p_2 = p, \quad -\mathbf{u}_1 = \mathbf{u}_2 = \mathbf{u}, \quad -\boldsymbol{\tau}_1 = \boldsymbol{\tau}_2 = \boldsymbol{\tau} = 2\eta \mathbf{d} \tag{64}$$

in (63) and obtain

$$X_N = \int_V dV (-p \nabla \cdot \mathbf{u} + \mathbf{u} \cdot \nabla p - \mathbf{u} \cdot (\nabla \cdot (2\eta \mathbf{d})))$$

$$+ \int_P dS \hat{\mathbf{U}} \cdot (\mathbf{n} \cdot (p \boldsymbol{\delta} - 2\eta \mathbf{d})). \tag{65}$$

As before, repeated use will be made of the divergence theorem. Also, the boundary conditions (9)–(11) are invoked. The first variation of (65) is

$$\delta X_N = -2 \int_V dV (\delta p \nabla \cdot \mathbf{u} + \delta \mathbf{u} \cdot (-\nabla p + \nabla \cdot (2\eta \mathbf{d}))), \tag{66}$$

so that, not unexpectedly, Eqs. (5) and (6) are recovered for the Newtonian case $\boldsymbol{\tau} = 2\eta \mathbf{d}$. It is immediate from (65) that the stationary value of X_N is the drag on the particle.

It will be useful to transform X_N into an alternative form. From (65) we obtain

$$X_N = \int_V dV (-2p \nabla \cdot \mathbf{u} + 2\eta \nabla \mathbf{u} : \mathbf{d}). \tag{67}$$

We switch to the shear rate tensor $\dot{\boldsymbol{\gamma}} = 2\mathbf{d}$ and the shear rate $\dot{\gamma}$ ($\dot{\gamma} \geq 0$) given by (see [8])

$$\dot{\boldsymbol{\gamma}}^2 = \frac{1}{2} \dot{\boldsymbol{\gamma}} : \dot{\boldsymbol{\gamma}} \tag{68}$$

and find

$$X_N = \int_V dV (-p Tr \dot{\boldsymbol{\gamma}} + \eta \dot{\boldsymbol{\gamma}}^2) \tag{69}$$

as an alternative to (65). We note that this is in fact Bird's functional ([3], Eqs. (12)–(15)) for the special case of a Newtonian fluid and no external force.

According to Pawlowski [2] and Bird [3], for the generalized Newtonian fluid we have available the functional

$$X_{GN} = \int_V dV (-p Tr \dot{\boldsymbol{\gamma}} + 2 \int_0^{\dot{\boldsymbol{\gamma}}} \eta(\dot{\boldsymbol{\gamma}}') \dot{\boldsymbol{\gamma}}' d\dot{\boldsymbol{\gamma}}'), \tag{70}$$

where the viscosity is shear rate dependent,

$$\boldsymbol{\tau} = \eta(\dot{\boldsymbol{\gamma}}) \dot{\boldsymbol{\gamma}}, \tag{71}$$

and a potential dependence on the 'third invariant' is discarded [8]. Well-known examples include the power law fluid and the Carreau-Yasuda model [8]. The original derivations showing that the functional (70) produces the correct governing equations employ the Euler-Lagrange equations. We prefer a direct approach. The first variation is

$$\delta X_{GN} = \int_V dV (-\delta p Tr \dot{\boldsymbol{\gamma}} - p Tr \delta \dot{\boldsymbol{\gamma}} + 2\eta(\dot{\boldsymbol{\gamma}}) \delta \dot{\boldsymbol{\gamma}}), \tag{72}$$

and using

$$2\dot{\boldsymbol{\gamma}} \delta \dot{\boldsymbol{\gamma}} = \dot{\boldsymbol{\gamma}} : \delta \dot{\boldsymbol{\gamma}}, \tag{73}$$

which follows from (68), we obtain

$$\delta X_{GN} = \int_V dV (-\delta p Tr \dot{\boldsymbol{\gamma}} - p Tr \delta \dot{\boldsymbol{\gamma}} + \eta(\dot{\boldsymbol{\gamma}}) \dot{\boldsymbol{\gamma}} : \delta \dot{\boldsymbol{\gamma}}). \tag{74}$$

We finally have

$$\delta X_{GN} = 2 \int_V dV (-\delta p \nabla \cdot \mathbf{u} + \delta \mathbf{u} \cdot (\nabla p - \nabla \cdot (\eta(\dot{\boldsymbol{\gamma}}) \dot{\boldsymbol{\gamma}}))), \tag{75}$$

so that (5) and (6) are indeed recovered for the generalized Newtonian fluid (71). However, there is no direct relation (in the sense of equality or proportionality) between the stationary value of (70) and the drag.

Returning to the two-label approach, we can formulate a functional with the generalized Newtonian drag as its stationary value. In analogy to (63) we put

$$X_{GN,2} = \int_V dV (p_1 \nabla \cdot \mathbf{u}_2 - \mathbf{u}_1 \cdot \nabla p_2)$$

$$+ \int_V dV (\frac{1}{2\eta_2} \boldsymbol{\tau}_1 : \boldsymbol{\tau}_2 - \boldsymbol{\tau}_1 : \mathbf{d}_2 + \mathbf{u}_1 \cdot (\nabla \cdot \boldsymbol{\tau}_2))$$

$$+ \int_P dS \hat{\mathbf{U}} \cdot (\mathbf{n} \cdot (p_2 \boldsymbol{\delta} - \boldsymbol{\tau}_2)) \tag{76}$$

with $\eta_2 = \eta(\dot{\boldsymbol{\gamma}}_2)$. Repeating the variational analysis we find for the fields with label 2 the generalized Newtonian Eqs. (5), (6) and (71), and the stationary value is the drag. For the fields with label 1 one obtains apart from (5) an equation of motion with an extra term (cf. (27)) and the stress tensor involves η_2 ,

$$\mathbf{0} = -\nabla p_1 + \nabla \cdot \boldsymbol{\tau}_1 + \nabla \cdot \boldsymbol{\pi}, \tag{77}$$

$$\boldsymbol{\pi} = \frac{1}{2\eta_2^2 \dot{\boldsymbol{\gamma}}_2} \frac{\partial \eta_2}{\partial \dot{\boldsymbol{\gamma}}_2} \boldsymbol{\gamma}_2 \boldsymbol{\tau}_1 : \boldsymbol{\tau}_2, \tag{78}$$

$$\boldsymbol{\tau}_1 = \eta_2 \dot{\boldsymbol{\gamma}}_1, \tag{79}$$

with an expected mix of fields with labels 1 and 2.

7. Concluding remarks

We have presented a variational principle for the Upper Convected Maxwell model. Using the principle we found a formula for the derivative of the drag with respect to the Deborah number for a particle in a duct. We contrasted the principle with the reciprocal theorem. Whereas the reciprocal theorem gives the drag as a volume integral involving the Stokesian stress tensor, the variational principle involves the stress from the adjoint equation. For low Deborah number both formulae give the correction to the Stokes drag as a volume integral involving

only the Stokesian rate-of-strain tensor. This is in line with second-order fluid theory. We also established a formal connection between the principle and a previously obtained functional for the generalized Newtonian fluid. Finally, we briefly discussed the incorporation of other rheological models into the variational framework.

It may be remarked that the variational principle seems more elaborate than the reciprocal theorem. For instance, the derivation of the low Deborah number formula for the drag (42) is shorter via the reciprocal theorem. It may well be that the potential advantage of the variational principle lies in finding approximations to the drag. The stationarity property ensures that first order deviations from the actual fields produce only second order deviations from the actual drag, enhancing the accuracy of the approximation (cf. the first observation at the end of Section 5). It remains to be seen whether the variational principle outlined in this paper is useful in this respect.

Declaration of competing interest

The author declares that he has no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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