



Korteweg stresses and admissibility criteria for shear banded flows



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ABSTRACT

Nonmonotone constitutive behavior leading to shear banding occurs in a number of fluids, such as wormlike micelles and clay suspensions. In general, shear banded flows are not unique. Higher order terms in the governing equations are often introduced to distinguish a preferred solution that arises as a steady state in the long term. In the literature on wormlike micelles, stress diffusion has been widely considered for this purpose.

In this paper, we discuss a different physical mechanism, based on interfacial energies and Korteweg stresses associated with them. It is shown how this criterion leads to a form of “equal area” rule.

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1. Introduction

Complex fluids including wormlike micelles, suspensions and colloids often show shear banding, i.e. the coexistence of high and low shear rates at the same shear stress. Theoretical efforts to model such fluids are often based on constitutive theories which predict a nonmonotone dependence of shear stress on shear rate. For such models, there exists a range of shear stresses for which shear bands can occur. In planar Couette flow, the location of shear bands is dependent on initial perturbations; in inhomogeneous shear flows such as circular Couette flow or Poiseuille flow, the shear band usually forms in the region of higher stresses. However, the precise location and the stress level at which the jump from low to high shear rate occurs is still nonunique and dependent on initial conditions. This prediction needs to be reconciled with the observation that steady flow behavior may instead show a “plateau,” i.e. a uniquely determined shear stress at which the transition from low to high shear rates occurs.

A criterion which has been widely suggested as a path to resolving this issue is based on stress diffusion, see for instance [7,12,16,19]. Say the constitutive law for the fluid postulates a stress consisting of a Newtonian “solvent” contribution and a viscoelastic stress \mathbf{T} given by a differential constitutive law of the form

$$\tau \frac{d}{dt} \mathbf{T} = \mathbf{G}(\nabla \mathbf{v}, \mathbf{T}). \quad (1)$$

Here d/dt stands for the material time derivative and τ is a relaxation time. Stress diffusion replaces this constitutive law by

$$\tau \frac{d}{dt} \mathbf{T} = \delta^2 \Delta \mathbf{T} + \mathbf{G}(\nabla \mathbf{v}, \mathbf{T}). \quad (2)$$

Here δ is a small length scale. The result of adding these diffusion terms is that the discontinuous shear banding transition is replaced by a smooth transition (over a length scale of order δ). “Admissible” steady flows are then those which arise in the limit $\delta \rightarrow 0$. We note that in numerical simulations of circular Couette flow in the literature the “plateau” is not entirely flat [14,20]; this is due to the finite width of the transition which causes the stresses at both ends to differ slightly. The diffusion coefficient used in these simulations is larger than what would be considered realistic.

There are basically two assumptions underlying the idea of stress diffusion:

1. Particles diffuse according to Fick’s law.
2. Stresses are determined as moments of a single particle distribution function, so, as they diffuse, particles carry their stresses with them.

These assumptions are quite reasonable for dumbbell models of dilute solutions, where the polymer molecules are presumed to interact only with a Newtonian solvent. I refer to [5] for a detailed derivation of stress diffusion resulting from Brownian forces acting on polymer molecules. However, such a picture is a stretch for the fluids in which shear banding actually occurs. It seems clear that diffusion laws ought to be more complicated than Fick’s law for a

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molecule that, for instance, is thought of as a kind of worm slithering through a network of tubes. The assumption that stresses are given in terms of a single particle distribution function also has limitations.

In addition, the mathematical consequences of stress diffusion are difficult to assess and may not always yield a desirable result. As is well explained in [12], the admissibility criterion obtained from stress diffusion amounts to finding a heteroclinic orbit in a dynamical system, which is far from simple and can be done explicitly only in limiting cases such as when the jump across the shear band is small. However, this situation may not be of much interest when in applications the jump in shear rate is typically several orders of magnitude. Moreover, we can identify situations where stress diffusion seems to be useless altogether. Consider for instance an elastic solid. In an elastic solid, the stress is a function of the deformation gradient \mathbf{F} ,

$$\mathbf{T} = \mathbf{H}(\mathbf{F}); \tag{3}$$

if we differentiate this, we obtain something similar to (1) above,

$$\frac{d\mathbf{T}}{dt} = \mathbf{G}(\nabla\mathbf{v}, \mathbf{F}). \tag{4}$$

Note that in a static deformation both sides of (4) are zero. So if we modify (4) by a stress diffusion term, we conclude that in a static deformation the diffusion term should also be zero. Therefore, the “prediction” of this criterion would be that all stress components should be continuous across the shear band. In general this cannot be satisfied.

In this paper, we shall consider an alternative criterion, which was originally proposed by van der Waals [18] and Korteweg [10] for the liquid–gas transition. In this theory, higher order terms do not appear in the constitutive law, but in the momentum equation. The theory is based on the postulate of an interfacial energy. In the case of the liquid–gas transition, the density has a jump across the interface, and smoothing of the interface is accomplished by introducing an interfacial energy which is assumed to depend on the density gradient. The interfacial energy becomes significant only when the density gradient is large. Usually, a quadratic dependence on the density gradient is assumed. Korteweg stresses are the forces which are associated with this interfacial energy. They depend on first and second gradients of density. The main achievement of the theory of van der Waals and Korteweg was that it explains Maxwell’s equal area rule for the liquid–gas transition. It also has been shown to give a microscopic explanation of interfacial tension.

The idea of an interfacial energy has been extended to the theory of mixtures [3] and to phase transitions in solid mechanics, which are associated with changes in crystal structure. An extensive literature has developed in this context, following the pioneering work of Ericksen [6]. In the context of elastic solids, interfacial energies may depend on higher order gradients of the deformation [2,3,13,17] or on an order parameter which replaces the concentration variable in mixture theories [8,9]. Such theories have also been connected [8,9] to sharp interface theories such as developed in [1]. Indeed, one of the main goals of developing regularized theories is to identify the selection of phase boundaries in equilibrium or to predict the velocity with which phase boundaries move when they are not in equilibrium.

We note that the authors in [16] try to motivate stress diffusion by the presence of an interfacial energy, without, however, establishing any rigorous connection. In contrast, it is well understood how Korteweg stresses are related to interfacial energies.

In this manuscript, we explore Korteweg stresses resulting from a tube misalignment energy. That is, we identify a tube conformation tensor which describes the deformation of tubes in theories of

entangled liquids, and we postulate an energy which is quadratic in the gradient of this conformation tensor.

For the sake of concreteness, we shall focus on parallel shear flows, and on a particular model leading to nonmonotone constitutive behavior, the PEC model of Larson [11]. We state the model in the form in which it is given in [15]. The extra stress is given by a Newtonian part and a “polymer” stress contribution:

$$\mathbf{S} = \eta(\nabla\mathbf{v} + (\nabla\mathbf{v})^T) + \mathbf{T}, \tag{5}$$

and \mathbf{T} is given in terms of a “conformation tensor” \mathbf{C} as

$$\mathbf{T} = \frac{k\mathbf{C}}{\text{tr}\mathbf{C} + \alpha}. \tag{6}$$

Finally, the conformation tensor satisfies the equation

$$\frac{d\mathbf{C}}{dt} = (\nabla\mathbf{v})\mathbf{C} + \mathbf{C}(\nabla\mathbf{v})^T - \epsilon(\text{tr}\mathbf{C} + \alpha)(\mathbf{C} - \mathbf{I}), \tag{7}$$

where \mathbf{I} is the identity matrix.

Larson obtains this model from a tube theory in which polymer molecules stretch only partially with their tubes. In this context, the tensor \mathbf{C} can naturally be interpreted as a tube conformation tensor. The natural adaptation of the Korteweg–van der Waals theory is the assumption of a “tube mismatch energy” with penalizes rapid changes in tube conformation. We shall assume that the energy density for this is of the form

$$W = \phi(\mathbf{C}, \nabla\mathbf{C}), \tag{8}$$

and that the dependence on $\nabla\mathbf{C}$ is quadratic:

$$W = \sum_{i,j,k,l,m,n} a_{ijklmn}(\mathbf{C}) \frac{\partial C_{ij}}{\partial x_k} \frac{\partial C_{lm}}{\partial x_n}. \tag{9}$$

As we shall see such an energy leads naturally to a Korteweg stress tensor which consists of a term linear in second derivatives of \mathbf{C} and a term quadratic in first derivatives.

A fully tensorial formulation would become quite complicated. There are six independent components of the symmetric tensor \mathbf{C} and three space directions, so there are eighteen different components of the gradient of \mathbf{C} . This leads to 171 coefficient in (9), which are related to each other by numerous symmetry constraints. The Korteweg stress would, as in the one-dimensional case discussed below, consists of a term linear in second derivatives of \mathbf{C} and a term quadratic in first derivatives.

We shall stick to the geometry of parallel shear flow. The flow is in the x -direction and varies with y . In the following we denote derivatives with respect to y by a prime and time derivatives by a dot. In shear flow, the PEC model leads to $C_{22} = C_{33} = 1$, $C_{13} = C_{23} = 0$, and we need to be concerned only with the C_{11} and C_{12} components. With $\kappa = u'$ denoting the shear rate, these satisfy the equations

$$\begin{aligned} \dot{C}_{11} &= 2C_{12}\kappa - \epsilon(C_{11} + 2 + \alpha)(C_{11} - 1), \\ \dot{C}_{12} &= \kappa - \epsilon(C_{11} + 2 + \alpha)C_{12}. \end{aligned} \tag{10}$$

We note that these equations are not changed by the Korteweg stresses. The interfacial energy will have the form

$$\begin{aligned} W &= a_1(C_{11}, C_{12})(C'_{11})^2 + a_2(C_{11}, C_{12})C'_{11}C'_{12} \\ &\quad + a_3(C_{11}, C_{12})(C'_{12})^2. \end{aligned} \tag{11}$$

Since this energy should not depend on the direction of shear, we assume that a_1 and a_3 are even functions of C_{12} , while a_2 is odd. Corresponding to this energy density is a Korteweg stress of the form

$$\begin{aligned} \tau &= b_1(C_{11}, C_{12})C''_{11} + b_2(C_{11}, C_{12})C''_{12} + b_3(C_{11}, C_{12})(C'_{11})^2 \\ &\quad + b_4(C_{11}, C_{12})C'_{11}C'_{12} + b_5(C_{11}, C_{12})(C'_{12})^2. \end{aligned} \tag{12}$$

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