Shear banding of semidilute polymer solutions in pressure-driven channel flow

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Shear banding is observed in many soft materials. We recently developed a two-fluid model for semidi- lute entangled polymer solutions by using the generalized bracket approach of nonequilibrium thermodynamics. This model assumes that Fickian diffusion and stress-induced migration generate a nontrivial velocity difference between the polymers and the solution, thereby resulting in shear band formation. A straightforward implementation of the slip boundary conditions is possible because the differential velocity is treated as a state variable. Numerical calculations showed obvious shear banding in the polymer concentration profile. Increasing the pressure gradient reduces the inhomogeneity of the concentration profile and moves the transition region toward the center of the channel. Moreover, the velocity deviates from the typical parabolic form and shows a plug-like profile with a low shear band near the center and a high one near the walls. The lack of hysteresis in the profiles of the volumetric flow rate calculated with the increasing and decreasing pressure gradient demonstrates the uniqueness of the solution. In addition, the flow rate exhibits a spurt at a critical pressure gradient, as experimentally observed for shear banding materials. The simplicity of the new model encourages us to analyze it in more complicated flows.

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1. Introduction

A rectilinear channel has simple geometry, which makes its flow problem a suitable benchmark problem for constitutive models and newly developed codes. Exact analytical solutions for a fully developed channel flow have been derived for various well-known differential viscoelastic fluid models, including the linearized and exponential forms of the Phan–Thien–Tanner [1–3], Giesekus [4,5], and Johnson–Segelmann [6] models. For instance, Oliveira and Pinho [1] found that the shear-thinning behavior reduces the wall shear stress and makes the velocity profiles flatter. Cruz et al. [3] investigated the effect of a nontrivial Newtonian solvent viscosity and observed that the spatial variation of the velocity field can be made flatter by increasing the ratio of the solvent viscosity to the total viscosity. In addition, the upper-convected Maxwell and Oldroyd-B models were analytically solved for a transient pressure-driven channel flow. They are now extensively used for validation purposes [7]. Depending on the choice of the model parameters, viscoelastic fluid models can exhibit intense temporal oscillations. Damped inertia-elastic shear waves travel across the channel and reflect back from the stationary walls. Duarte et al. [8] found that the transient response is longer for larger elasticity numbers, and the frequency of the oscillations is higher. Furthermore, shear thinning reduced the time required to reach a steady state. The presence of a large Newtonian solvent contribution leads to a smaller oscillatory frequency of the response as well as an attenuation of the oscillation peak [8–10]. Slip along the channel is important, as it is widely observed under strong deformations of viscoelastic materials. Meanwhile, Ferrás et al. [11] analytically solved the Giesekus model and a simplified version of the PTT model under linear and nonlinear Navier, Hatzikiriakos, and asymptotic slip conditions. They showed that a unique steady-state solution always exists for the four phenomenological slip models considered for a simplified PTT model. For the Giesekus model, the existence of the solution can be numerically proven for some cases with slip if no physical solution exists because of the Weissensberg number restrictions in the no-slip condition.

Shear banding, which is defined as localized bands with different shear rates, is ubiquitously observed in soft materials. However, its underlying mechanisms are not always the same. While the shear banding instability of wormlike micelles is caused by a combination of reptation and micellar breakage, that of semidilute polymers is still an open issue of debate. Shear banding in complex fluids is reviewed in [12–14]. Several experimental studies focused on the shear banding phenomenon in Poiseuille flows. Particle image velocimetry (PIV) experiments performed on wormlike micelles in microchannels [15], regular channels [16], and capillar-
ties [17,18] revealed that a spurt is evident in the rapid increase in the velocity or flow rate at the critical pressure gradient. The velocity profiles exhibit Newtonian behavior at low shear rates. Some systems form an apparent slip below the onset of the spurt. Kim et al. [15] noted that the recorded slip velocity may be an artifact of very thin shear-banding layers near the walls, which are too thin to be optically resolved. The velocity changes from a parabolic profile to a plug-like one during the transition to the shear banding regime. Furthermore, the interface between the shear bands was spatially undulating [19]. Experimental evidence also suggests that the velocity profile of colloidal particles shows a plug-like shape as a result of shear-induced migration [20]. By performing PIV in microchannels, Degré et al. [21] observed that the maximum velocity for shear-thinning, non-shear-banding polymer solutions superlinearly increases with the applied pressure gradient in the nonlinear viscoelastic regime. The velocity profile slightly departs from the parabolic profile of the Newtonian fluids and exhibits a depletion layer in the micrometer range. The flow curve of the polymer melts shows a spurt and hysteresis in pressure-driven experiments. The wall slip in polymer melts, particularly, is extensively studied because of its potential influence on extrusion instabilities [22]. The extent to which semidilute entangled polymer solutions exhibit the above-described phenomena is currently unclear because of the lack of experimental data.

McLeish and Ball [23] conducted the very first numerical study that relates the spurt in a Poiseuille flow to the shear banding phenomenon. They used an improved version of the Doi-Edwards model, which also incorporates stress contributions with shorter relaxation times than the reptation time of a single polymer chain, to capture the rheology of monodisperse polymer melts. This model exhibits a nonmonotonic steady flow curve under homogeneous flow conditions. Hence, they were able to capture the hysteretic loops in the profile of the volumetric flow rate plotted against the applied pressure gradient. Radulescu and Olmsted [24] also published an early work on shear banding using nonlocal stress diffusive terms. Two distinct shear bands were found below the critical point of monotonicity for the Johnson–Segalman model in the case of an inertia-less Poiseuille flow. Many years later, Fielding and Wilson [25] performed a fully nonlinear stability analysis of the same model in a pressure-driven channel flow. They applied small perturbations in the flow/flow-gradient plane and flow-gradient/vorticity plane and showed that the initially flat interface was unstable with respect to the growth of undulations along it. The Vasquez–Cook–McKinley (VCM) two-species model for wormlike micelles was also examined [26]. The authors showed an onset of shear and concentration banding above a critical pressure gradient. The interface between the bands initially forms near the walls, and then moves toward the center. The VCM model predicts a jump in the volumetric flow rate at the critical pressure drop and hysteresis, as experimentally observed for wormlike micelles. Subsequently, these authors investigated the linear stability of the VCM model and suggested that the spectrum of the unstable modes is reduced if the interface between the bands is smoothed by using a larger diffusivity constant or smaller characteristic channel dimensions [27]. Thus far, shear banding in pressure-driven flows has only been predicted for one-fluid viscoelastic constitutive models showing a nonmonotonic homogeneous flow curve. Such models are well known to be unable to predict steady-state bands if the curve is strictly monotonic. Therefore, a more complex two-fluid model, such as the one used in the present work, is required to examine the shear banding instability of semidilute entangled polymer solutions [28,29]. Ianniruberto et al. [30] solved Doi and Milners’ two-fluid theory for semidilute entangled polymer solutions for a pressure-driven channel flow. They found stress–induced migration of the polymers toward the center. However, their predictions were limited to pressure gradients smaller than the shear banding regime.

Germann et al. [31,32] used the generalized bracket approach of nonequilibrium thermodynamics to develop a multifluid framework that would account for the Fickian diffusion and stress–induced migration in viscoelastic materials. The differential velocities are treated as state variables. Hence, the additional boundary conditions arising from the diffusive derivative terms can be directly imposed with respect to these variables. This description is advantageous because it allows for a straightforward formulation of the boundary conditions. For instance, no-slip and no-flux conditions translate into the requirements that the tangential and normal components of the differential velocities must vanish at the boundaries. The standard approach used in the two-fluid description to impose the additional boundary conditions arising from the diffusive derivative terms is to require no flow of concentration and construct the stress/conformation conditions, such that the total flux vanishes at the boundaries [33–36]. This approach works well for mixtures of two fluids that exhibit no slip along the walls. However, it cannot be applied that easily if wall slip, mixtures of more than two phases, and/or flows in more complicated geometries are considered. Hooshyar and Germann [37] used this framework to develop a new two-fluid model for semidilute entangled polymer solutions.

Several experimental studies reported that concentrated solutions of high-molecular-weight polymers subjected to shear flow can form spatial inhomogeneities in the concentration profile [38–40]. Based on this evidence, Leal’s group [36,41] formulated a two-fluid Rolie–Poly model and showed that a realistic constitutive model for the stress and concentration coupling is required to predict shear bands at steady state. Hooshyar and Germann [37] developed a new model based on the same idea using the generalized bracket approach of nonequilibrium thermodynamics. A nonlinear Giesekus relaxation is used in the conformation tensor equation of the new model to capture the overshoot occurring during the rapid start-up of simple shear flow. The Giesekus relaxation is an appropriate choice because it accounts for the hydrodynamic interactions between the polymeric constituents in a concentrated solution. An additional relaxation term similar to that used in the Rolie–Poly model accounting for convective constraint release (CCR) and chain stretch were proposed using nonequilibrium thermodynamic arguments to predict the upturn of the flow curve at high shear rates. While our model is more phenomenological than the two-fluid Rolie–Poly model, it fully satisfies the fundamental laws of thermodynamics. In our previous study, the behavior of the new model was analyzed in a cylindrical Couette flow. The results showed that the steady-state solution is unique for different initial conditions and independent of the applied deformation history. Furthermore, we found that steady banding is associated with the term in the time equation of the differential velocity that accounts for the stress-induced migration of the polymers.

This study aims to investigate the new model in a rectilinear channel flow driven by a pressure gradient. The remainder of this paper is organized as follows: Section 2 presents the new thermodynamic model; Section 3 introduces the flow problem and numerical procedure; Section 4 presents and discusses the computational results; and Section 5 presents the conclusions of this study.

2. Two-fluid Polymer Model

In this section, we introduce the equations of our two-fluid polymer model. Note that all terms used for this model were derived using the generalized bracket approach of nonequilibrium thermodynamics. The complete derivation can be found in [37]. The total system considered in this model is assumed to be closed,
isothermal, and incompressible. This system consists of the two following components: one species of polymeric constituents and a viscous solvent. We define the following variables for the polymeric species: mass density $\rho_p$; momentum density $\mathbf{m}^p = \rho_p \mathbf{v}^p$, where $\mathbf{v}^p$ is the velocity field; and $\mathbf{c}$, which is the conformation tensor representing the average second moment of the end-to-end connection vector of the polymeric constituents. The polymer number density is given as $n_p = (\rho_p/M_p)N_k$, with $M_p$ being the molecular weight of the polymer and $N_k$, the Avogadro constant. The following variables are defined for a viscous solvent: mass density $\rho_s$ and momentum density $\mathbf{m}^s = \rho_s \mathbf{v}^s$, with $\mathbf{v}^s$ being the velocity field. The time evolution equations of the state variables are as follows:

$$\frac{\partial \mathbf{v}}{\partial t} = -\rho \mathbf{v} \cdot \nabla \mathbf{v} - \nabla p + \nabla \cdot \mathbf{\sigma},$$  

(1)

$$\frac{\partial \rho_s}{\partial t} + \frac{\partial \rho p}{\rho} \left( \frac{\partial \mathbf{v}}{\partial t} + \nabla \cdot \mathbf{v} \right) = -\nabla \cdot \rho_s \mathbf{v} + \nabla \cdot \mathbf{\sigma},$$

(2)

$$\frac{\partial \mathbf{c}}{\partial t} = -\mathbf{v} \cdot \nabla \mathbf{c} + \mathbf{c} \cdot \nabla \mathbf{v} + \left( \nabla \mathbf{v} \right)^T \cdot \mathbf{c} - \frac{1}{\lambda_1} \left[ (1-\alpha)I + \alpha \frac{K}{K_g} \mathbf{c} \right] \cdot \left( \mathbf{c} - \frac{k_g K}{K} I \right) - \frac{1}{\lambda_2} \left[ \text{tr} \left( \frac{K}{K_g} \mathbf{c} \right) - 3 \right] \mathbf{c} - \frac{k_g K}{K} I + D_{\text{mloc}} \left( \mathbf{c} \cdot \nabla \left( \mathbf{v} \cdot \mathbf{\sigma} \right) + \left[ \nabla \left( \mathbf{v} \cdot \mathbf{\sigma} \right) \right]^T \cdot \mathbf{c} \right).$$

(3)

Eq. (1) is the Cauchy momentum balance, where $\rho = \rho_s + \rho_p$ represents the total mass density; $t$ is time; $p$ is pressure; $\mathbf{v}$ is the mass-averaged velocity of the polymer solution; and $\mathbf{\sigma}$ is the extra stress tensor associated with the polymer solution. Eq. (2) gives the time evolution equation for the differential velocity $\Delta \mathbf{v}$, $k_g$ denotes the Boltzmann constant; $T$ is the absolute temperature; $\eta_s$ is the viscosity of the solvent; and $\mathbf{\sigma}$ is the extra stress associated with the polymer. The divergence of the tensor $\mathbf{\sigma}$ accounts for the stress-induced migration. The spatial gradients of the number densities associated with the polymer and solvent describe the Fickian diffusion. The local diffusivity constant $D$ controls the diffusion between the polymeric constituents and the solvent. The value of this parameter has no effect on the steady-state solution. However, the time to reach the steady state increases for smaller values [37]. The last term was added to facilitate the numerical computations of the strong boundary layers arising in the differential velocity component tangential to the wall in the presence of slip. This term is obtained as follows by adding extra viscous dissipation to the dissipation bracket:

$$[F, H] = -\int_{\Omega} \frac{\eta_{\text{extra}}}{2} \left[ \nabla_a \left( \frac{\delta F}{\delta (\Delta m^p)} \right) + \nabla_b \left( \frac{\delta F}{\delta (\Delta m^s)} \right) \right] \times \left[ \nabla_a \left( \frac{\delta H}{\delta (\Delta m^p)} \right) + \nabla_b \left( \frac{\delta H}{\delta (\Delta m^s)} \right) \right] d^3x,$$

(5)

where $\Omega$ is the flow domain; $F$ is an arbitrary functional depending on the state variables; $H$ is the Hamiltonian; $\Delta \mathbf{m}^p = (\rho_s/\rho) \Delta \mathbf{m} - (\rho_p/\rho) \mathbf{m}$ is the differential momentum density defined in Hooshyar and Germann [37]; and $\eta_{\text{extra}}$ is the dynamic viscosity controlling the sharpness of the boundary layer. The additional viscous dissipative term only appears in the time evolution equation for the differential velocity because the derivatives in Eq. (5) are taken with respect to the differential momentum density. Eq. (3) gives the time evolution equation for the polymer number density. The terms of the equation form the material derivative and account for the fact that the polymer concentration can vary locally. Eq. (4) gives the time evolution equation for the conformation of the polymer, where $\alpha$ is the Giesekus anisotropy factor, and $K$ is the Hookean spring constant associated with the polymer. The left-hand side along with the first three terms on the right-hand side constitutes the upper-convected time derivative. The fourth term on the right-hand side corresponds to the Giesekus relaxation, accounts for the hydrodynamic interactions, and generates a transient overshoot of the shear stress. The fifth term on the right-hand side of Eq. (4) is a nonlinear relaxation term added to generate the upturn of the flow curve at high shear rates. This term has a similar structure as that used in the Rolie-Poly model for accounting for convective constraint release, including chain stretch [42]. The power-law prefactor $[K/(k_g T)\text{trc} - 3]^0$, being a scalar function of the trace of the conformation tensor and thus a measure of polymer stretch, is used to describe the monotonic increase of the steady-state flow curve. This factor is appropriate because it allows for an upturn without the need for a solvent contribution [37]. We obtain $[\text{tr} \mathbf{\sigma}^2(\eta k_g K)]^0$ if we rewrite this factor in terms of the extra stress associated with the polymer. Assuming a constant polymer number density, this stress-dependent expression exactly reduces to the scalar CCR-function of the one-fluid Rolie-Poly model [42]. In the last term on the right-hand side of Eq. (4), the nonlocal diffusivity $D_{\text{mloc}}$ controls the smoothness of the profiles and guarantees a unique solution. Opposing the standard form of the Laplacian of the conformation tensor, this term can be formulated within the generalized bracket approach. The corresponding dissipation bracket can be found in [37]. Note the similarities between the stress diffusive terms appearing in Eqs. (2) and (4). An explicit expression for the differential velocity can be obtained from Eq. (2) in the absence of inertia. Inserting this expression into Eq. (4) yields stress diffusive terms with the same structure as those we added. The aim of our previous work was to develop a simple model for use in complex flows. Therefore, we decided to directly add a nonlocal term to the conformation tensor. Alternatively, the total system energy could be augmented by a nonlocal expression. However, we need to relax the assumption of incompressibility to properly implement such an expression in our two-fluid framework [43]. This move would make the numerical solution of the resulting model equations much more challenging because the pressure would not anymore be a projector operator of the velocity derivative in the divergence-free space and must be explicitly defined in terms of the state variables [44].

The abovementioned set of time evolution equations is closed by an explicit expression for the extra stress as follows:

$$\mathbf{\sigma} = \mathbf{\sigma}^0 + \mathbf{\sigma}^4 = \eta_s (K \mathbf{c} - k_g K I) + \eta_s (\nabla \mathbf{v} + (\nabla \mathbf{v})^T) \mathbf{c},$$

(6)

The first term on the right-hand side of Eq. (6) accounts for the viscoelastic stress of the polymer, whereas the second one accounts for the contribution of the viscous solvent. The total and differential velocities in our two-fluid framework are defined as follows:

$$\mathbf{v} = \frac{\partial \rho}{\rho} \rho^p \mathbf{v}^p + \frac{\partial \rho}{\rho} \rho^s \mathbf{v}^s,$$

(7)

$$\Delta \mathbf{v} = \mathbf{v}^p - \mathbf{v}^s.$$  

(8)
Consequently, the phase velocities can be recovered from the total average and differential velocities as follows:

$\mathbf{v}^0 = \mathbf{v} + \frac{\rho_s}{\rho} \Delta \mathbf{v}$,

(9)

$\mathbf{v}^s = \mathbf{v} - \frac{\rho_s}{\rho} \Delta \mathbf{v}$.

(10)

The analytical solution of $n_p = n_0^p$ and $c = (k_T^p/K) \mathbf{I}$ in the equilibrium state of rest ($\mathbf{v} = 0$ and $\Delta \mathbf{v} = 0$) can be obtained.

3. Flow problem

We consider a one-dimensional Poiseuille flow through a straight channel. Fig. 1 shows a schematic of the problem, where $H$ and $L$ denote the height and length of the channel, respectively. The inlet and outlet effects can be neglected because we assume $H \ll L$. Furthermore, any dependence on the $z$-direction is ignored. The Cartesian coordinate system is used as the reference frame with origin at the centerline. The walls are kept stationary, whereas a nonzero pressure gradient $\Delta p$ is applied in the $x$-direction.

The flow problem can be solved only for the upper half of the channel to avoid unnecessary computations because the flow is symmetric with respect to the centerline. The symmetry of the state variables can be guaranteed by using the following conditions:

\[
\frac{\partial v_x}{\partial y} = \frac{\partial \Delta v_x}{\partial y} = \frac{\partial \Delta v_y}{\partial y} = \frac{\partial c_{xx}}{\partial y} - \frac{\partial c_{xy}}{\partial y} = 0 \\
\frac{\partial n_p}{\partial y} = 0 \quad \text{at} \quad y = 0,
\]

(11)

\[
c_{xy} = 0 \quad \text{at} \quad y = 0.
\]

(12)

Symmetry requires the partial derivatives of the total velocity, differential velocity, normal components of the stress tensor, and polymer number density with respect to the channel position to be zero at the centerline. Furthermore, the value of the total momentum balance Eq. (1) and the maximum of the total velocity at the centerline require the shear stress and thus the $xy$-component of the conformation tensor there to be zero. The normal components of the total and differential velocities are required to be zero at the wall to guarantee no influx of the material through the walls:

$\mathbf{v} = \Delta \mathbf{v} = 0 \quad \text{at} \quad y = H/2$.

(13)

The tangential components of the total and differential velocities are set to zero at the wall if the wall has a no-slip condition:

$\mathbf{v}_x = \Delta \mathbf{v}_x = 0 \quad \text{at} \quad y = H/2$.

(14)

We also considered the case of slip along the walls. We used the standard linear Navier condition [11], which relates the wall shear stress to the wall velocity as follows, to illustrate how to account for the slip in our two-fluid framework:

$\mathbf{v}^s_x = -k_p \sigma^p_{xy}$,

(15)

$\mathbf{v}^s_y = -k_p \sigma^p_{xy}$.

(16)

where the constants $k_p$ and $k_s$ control the slip magnitude. These constants must be positive for the coordinate system placed as shown in Fig. 1. The following expressions for the tangential components of the kinematic state variables can be obtained if we insert Eqs. (15) and (16) into Eqs. (7) and (8):

$\mathbf{v}_x = \frac{\rho_s}{\rho} \mathbf{v}^s_x + \frac{\rho_s}{\rho} \mathbf{v}^s_x = -k_p \frac{\rho_s}{\rho} \sigma^p_{xy} + k_p \frac{\rho_s}{\rho} \sigma^s_{xy} \quad \text{at} \quad y = H/2$.

(17)

$\mathbf{v}_y = \frac{\rho_s}{\rho} \mathbf{v}^s_y = -k_p \frac{\rho_s}{\rho} \sigma^p_{xy} - k_p \frac{\rho_s}{\rho} \sigma^s_{xy} \quad \text{at} \quad y = H/2$.

(18)

As evident from Eqs. (17)-(18), we can easily impose wall slip on each phase by imposing the corresponding conditions on the total and differential velocities. Note that the higher-order derivatives appearing in the last term of Eq. (4) require special treatment at the boundaries [32]. The conformation diffusion should vanish at the solid boundaries within a distance less than the radius of gyration because of the local surface effects and because the diffusivity is essentially proportional to the normal thickness of the polymer molecules. The thickness becomes zero as these become flat to fit next to the surface. A detailed explanation can be found in Mavrantzas and Beris [45], where the main reason, namely, the surface acting as a barrier prohibiting many internal conformations, is mentioned along with an exact analysis for cytoplasm. These researchers showed that this quantity is proportional to the normal to the wall thickness of the polymer chains and goes to zero at the wall. Their findings are in excellent quantitative agreement with the Monte Carlo results of Fitzgibbon and McCullough [46] and the molecular dynamics simulations of Bitsanis and Hadzioannou [47]. In this manner, the use of any boundary conditions on the conformation tensor, which are arbitrary in our opinion, can be avoided. The best alternative would be to conduct a microscopic analysis down to the monomer length scale next to the wall, which would substantially increase the complexity of the model and its numerical solution. We do not make any assumption here on the shape of $D_{nonloc}$ and set this parameter equal to zero at the walls and to one elsewhere for simplicity. This approach works well as long as the gradients of the conformation tensor are not too high.

We work with dimensionless quantities, hereafter. The location across the gap is scaled by the channel height, $\mathbf{y} = y/H$. Time is scaled by the characteristic relaxation time, $\tilde{t} = t/\lambda_1$. The extra stress is scaled as $\tilde{\sigma} = \sigma / \tilde{G}_0$, while the conformation tensor associated with the polymer is scaled as $\tilde{\xi} = (K/k_T^p) c$. The polymer and solvent number density variables are normalized using the values at the equilibrium state as $\tilde{\mathbf{n}}_p = n_0^p / \rho_0^p$ and $\tilde{\mathbf{n}}_s = n_0^s / \rho_0^s$, respectively. The dimensionless parameters with respect to these scalings are the pressure gradient $\tilde{p}_x = \Delta \mathbf{p} / \rho \tilde{G}_0$; elasticity number $\tilde{E} = G_0 \lambda_1^2 / \rho H^2$; ratio of the molecular weight of the solvent to that of the polymer, $\chi = M_s / M_p$; viscosity ratio $\tilde{\eta} = \eta_0 / \eta_0^p$, where $\eta_0^p = G_0 \lambda_1$ is the zero shear viscosity; boundary layer constant $\tilde{\xi} = \xi_{extra} / \eta_0$; and ratio of the characteristic relaxation times $\tilde{\epsilon} = \lambda_1 / \lambda_2$. By assuming an initially uniform polymer concentration in the flow field, the polymer concentration corresponds to the initial local polymer concentration, and is, thus, given in weight percent by $\mu = \tilde{\mathbf{n}}_p^3 / \tilde{\mathbf{n}}_s^3 + \chi \tilde{\mathbf{n}}_s^3$. The dimensionless diffusion coefficients are defined as $\tilde{D} = D \lambda_1 / H^2$ and $\tilde{D}_{nonloc} = D_{nonloc} \lambda_1 / H^2$. The dimensionless form of the model equations can be found in Appendix A.

The flow problem was solved using the numerical procedure described in Hooshyar and Germann [37]. We used a Chebyshev pseudospectral collocation method [48,49] with 200 collocation points for spatial discretization and a second-order Crank–Nicolson scheme [50] for temporal discretization. The nonlinear system of discretized algebraic equations was solved at each time step using an inverse-based incomplete lower–upper (ILU) preconditioned Newton–Krylov solver [51,52].
4. Results

In this section, we analyze the behavior of the new model comprising time evolution Eqs. (1)-(4), the explicit expression of the extra stress tensor provided in Eq. (6), and the definitions of the phase velocities provided in Eqs. (9)-(10) in a pressure-driven channel flow. First, we start with no slip, where the tangential components of the total and differential velocities are required to be zero at the wall, as formulated in Eq. (14). The remaining boundary conditions are provided in Eqs. (11)-(13).

First, we solved the Oldroyd-B model for the flow problem described in Section 3 and compared the numerical results with the transient analytical solution of Waters and King [7] to validate the numerical code. The Oldroyd-B model is a limiting case of the two-fluid model obtained by setting \( \alpha = \epsilon = \tilde{D} = \tilde{D}_{\text{nonloc}} = 0 \). Fig. 2 shows the temporal evolution of the magnitude of the shear stress at the wall, which is manifested by damped oscillations converging to its steady-state value. The results are in excellent agreement with the analytical solution, thereby confirming the validity and accuracy of the numerical code. Furthermore, we observed that a larger pressure gradient leads to an increase in the average magnitude of the wall shear stress and amplitude of the oscillations (see Fig. 2a). Increasing \( E^{-1} \) has no effect on the steady state. Inertia only decreases the frequency of the oscillations (Fig. 2b).

Second, we present how the model parameters affect the solution of the two-fluid model presented in Section 2. The approximate values of the model parameters were determined in Hoo shyar and Germann [37] by fitting to the steady-state shear rheology of a 10 wt./wt.\% (1.6M) polybutadiene solution [53]: \( \alpha = 0.73, \epsilon = 0.0025, q = 1.46, \chi = 10^{-1} \), and \( \beta = 10^{-3} \). The corresponding constitutive curve for the homogeneous shear flow can be found in this paper. The boundary layers in the no-slip case are less steep. Therefore, smoothing the profiles was not necessary, and the boundary layer constant was simply set to zero. Fig. 3 shows the temporal evolution of the magnitude of the wall shear stress for different values of the anisotropy factor \( \alpha \). The most intense oscillation is obtained for \( \alpha = 0 \), as expected from Duarte et al. [8]. Increasing this parameter dampens the oscillations faster. As expected, the steady-state value of the wall shear stress is slightly smaller for a larger value of \( \alpha \) (i.e., for greater shear thinning). We use \( \alpha = 0.73 \) for all subsequent calculations.

Fig. 4 shows the influence of the local diffusivity constant on the temporal evolution of the absolute value of the shear stress and the polymer number density at the wall. Fig. 4a shows that neither the transient evolution of the wall shear stress nor its steady state significantly varied with the value of \( \tilde{D} \). Fig. 4b shows that the polymer concentration at the wall needs more time for smaller values of \( \tilde{D} \) to reach the steady state, which is independent of this parameter. Increasing the value of the local diffusivity reveals two undershoots in this curve. The first undershoot occurs at \( \tilde{t} = 0.05 \), which corresponds to the time at which the oscillations of the shear stress and the x-component of the total and differential velocities are totally damped. The second undershoot for \( \tilde{D} \geq 0.1 \) corresponds to the fact that the velocity profile increases to a temporary maximum at \( \tilde{t} \geq 3 \) (Fig. 5b).

Fig. 5 presents the effect of diffusion on the temporal evolution of the total velocity. In Fig. 5a, we observe that the local velocity for \( \tilde{D} = 10^{-3} \) monotonically increases at each point in the flow domain to the corresponding value of the steady state. The velocity at the centerline for \( \tilde{D} = 10^{-1} \) increases to a temporary maximum, and then decreases to the steady-state profile (Fig. 5b). However, we do not expect this phenomenon to be observed experimentally because the value of \( \tilde{D} \) is extremely large in this case.

Fig. 6 shows how the nonlocal diffusivity influences the solution. The parameter \( \tilde{D}_{\text{nonloc}} \) does not substantially affect either the transient or the steady-state solution of the wall shear stress (Fig. 6a). The profiles of the polymer number density obtained for different values of \( \tilde{D}_{\text{nonloc}} \) reach the steady state at approximately the same time (Fig. 6b). However, Fig. 6c shows that a larger value of \( \tilde{D}_{\text{nonloc}} \) leads to a more uniform concentration profile in the steady state. The kinks separating the bands in this curve become closer to the centerline as the nonlocal diffusivity decreases because of the lower stress diffusion. Interestingly, the value of \( \tilde{D}_{\text{nonloc}} \) does not greatly affect the steady-state velocity across the gap, as shown in Fig. 6d. We plot the x- and xy-components of the conformation tensor in the vicinity of the upper wall to confirm that the selected shape of the nonlocal diffusivity results in a smooth near-wall dynamics (Fig. 7).

Fig. 2. Temporal evolution of the magnitude of the wall shear stress calculated for the Oldroyd-B model with \( \beta = 10^{-5} \) and validation with the analytical solution using (a) different values of the pressure gradient with \( E^{-1} = 10^{-5} \) and (b) different reciprocal elasticities with \( \sigma_1 = -10 \).

Fig. 3. Temporal evolution of the magnitude of the shear stress at the wall calculated for the two-fluid model using different values of \( \alpha \). The other nontrivial values of the model parameters used in the calculation are \( E^{-1} = 10^{-5} \), \( \beta = -10 \), \( \epsilon = 0.0025 \), \( q = 1.46 \), \( \beta = 10^{-3} \), \( \chi = 10^{-1} \), and \( \tilde{D} = \tilde{D}_{\text{nonloc}} = 10^{-1} \).
Fig. 4. Effect of $\mathcal{D}$ on the (a) temporal evolution of the magnitude of the wall shear stress and the (b) temporal evolution of the polymer number density at the wall. The other nontrivial values of the model parameters are $E^{-1} = 10^{-3}$, $\tilde{R} = -10$, $\alpha = 0.73$, $\epsilon = 0.0025$, $q = 1.46$, $\beta = 10^{-3}$, $\chi = 10^{-1}$, and $\mathcal{D}_{\text{nonloc}} = 10^{-3}$.

Fig. 5. Temporal evolution of the velocity profile with (a) $\mathcal{D} = 10^{-3}$ and (b) $\mathcal{D} = 10^{-1}$. The other nontrivial values of the model parameters are $E^{-1} = 10^{-3}$, $\tilde{R} = -10$, $\alpha = 0.73$, $\epsilon = 0.0025$, $q = 1.46$, $\beta = 10^{-3}$, $\chi = 10^{-1}$, and $\mathcal{D}_{\text{nonloc}} = 10^{-3}$.

Fig. 6. Effect of $\tilde{D}_{\text{nonloc}}$ on the (a) temporal evolution of the wall shear stress magnitude, (b) temporal evolution of the polymer number density at the wall, (c) steady-state profile of the polymer number density across the gap, and (d) steady-state profile of the velocity across the gap. The other nontrivial values of the model parameters are the same as those given in the caption of Fig. 5a.
Figs. 8a–d show the effect of increasing the absolute value of the pressure gradient on the steady-state profiles of the velocity, shear stress, first normal stress difference, and polymer number density across the gap, respectively. The velocity profile decreases from the centerline to the walls with a low shear band near the center and a high one near the walls. The sharp kink separating these bands is considerably smoother than that predicted by the VCM model [26] for wormlike micelles. No sharp transition is obtained here even if $D_{\text{nonloc}} = 0$. The velocity profile for $P_k = -1$ is linear. The profile becomes plug-like as the magnitude of the pressure gradient further increases. Moreover, the maximum value of the velocity decreases. As required by the total momentum balance, the magnitude of the shear stress linearly increases from zero at the centerline to its maximum at the wall, where this value is larger for the larger absolute values of the pressure gradient. The first normal stress difference monotonically increases from the center to a maximum value at the walls, which is larger for the larger absolute values of the pressure gradient. This profile is different from that predicted by the VCM model, which exhibits a local maximum at the location of the kink because of the flow-induced breakage of the wormlike micelles (c.f., Fig. 12 of Cromer et al. [26]). The concentration bands shown in Fig. 8d are predicted by the two-fluid model for the same range of pressure gradients, where the velocity profile assumes a plug-like shape. Increasing the magnitude of the pressure gradient reduces the inhomogeneity of the concentration profile and moves the transition region toward the centerline. The polymer concentration is higher at the center than at the wall, which is in agreement with the predictions by Ianniruberto et al. [30] for semidilute entangled polymer solutions below the onset of shear banding. The decrease of the polymer concentration already occurs where the velocity profile is plug-like.

The volumetric flow rate is calculated using different values of the pressure gradient with $D_{\text{nonloc}} = 10^{-3}$, which results in a profile with a spurt at a critical value of the pressure gradient $P_{K,cr} \simeq 1.5$. The agreement of the ramp-up and ramp-down curves shown in Fig. 9a confirms the uniqueness of the solution. The nonuniqueness of the results indicated by the hysteresis in constitutive mod-
els showing a nonmonotonic flow curve under homogeneous conditions is not observed here. This discrepancy is related to the different underlying mechanisms of the shear band formation and must be experimentally verified in the future. Next, we examine the influence of the nonlocal diffusivity constant on the ramp-up test shown in Fig. 9b. The critical pressure gradient is not affected by this parameter. Furthermore, the value of the nonlocal diffusivity slightly changes the value of the flow rate in the region of the spurt \((-3 < \tilde{p}_x \leq -1.5\). The smallest nonlocal diffusivity leads to the largest flow rate in the shear banding regime, whereas the opposite behavior is observed in the linear viscoelastic regime.

Fig. 10 shows the effect of \(\tilde{D}_{nonloc}\) on the profile indicating the relation between the pressure gradient and the location of the kink separating the shear bands. We find that increasing the magnitude of \(\tilde{p}_x\) moves the kink toward the centerline. The inset of Fig. 10 shows that the value of \(\tilde{D}_{nonloc}\) only has a minor influence on this profile for \(\tilde{p}_x \geq -40\). As already discussed, in this region and at fixed pressure gradient, the kink is closer to the wall for a larger nonlocal diffusivity. However, a significant impact is observed for large absolute values of the pressure gradient \(\tilde{p}_x \leq -90\). This finding is related to the fact that the shear bands fade out at smaller absolute values of \(\tilde{p}_x\) for larger \(\tilde{D}_{nonloc}\).

Finally, we consider the effect of slip using Eqs. (17)-(18). A nontrivial positive value of the boundary layer constant \(\xi\) had to be used to be able to numerically resolve the steep gradients of \(\Delta v_x\). Fig. 11 shows the x-component of the total velocity (left column) and the differential velocity (right column) across the gap for two different pressure gradients, namely, \(\tilde{p}_x = 10\) (top figures) and \(\tilde{p}_x = 100\) (bottom figures). The steady-state differential velocity in the y-direction is zero. Therefore, we do not show the profile of this component. Note that all components of the vector \(\Delta \mathbf{v}\) in the no-slip case are zero at the steady state. We note that the parameter \(k_s\) that controls the amount of wall slip of the solvent has no significant effect if the results of \(k_p = k_s = 50\) are compared with those of \(k_p = 50\) and \(k_s = 0\). However, increasing the value of \(k_p\), the polymer slip results in a vertical downward shift of the whole profile of \(\tilde{v}_x\), thereby leading to a larger wall slip velocity. Interestingly, the parameter \(\tilde{p}_x\) has no effect on the shape of the profiles; it only increases the magnitudes of \(\tilde{v}_x\) and \(\Delta \tilde{v}_x\).

We examine the influence of this quantity below to demonstrate that the selected value of \(\xi = 10^{-3}\) had no effect on the results discussed in the preceding paragraph. Figs. 12a–b show the profiles of the polymer number density and differential velocity, respectively, in the x-direction across the channel for different \(\xi\) values. We observe that the profiles of \(\tilde{n}_p\) are not affected. Up to moderate values (i.e., for \(\xi \leq 10^{-2}\), the boundary layer constant has no influence on the profiles of \(\Delta \tilde{v}_x\) in the region inside the channel. However, decreasing the \(\xi\) value leads to steeper gradients near the solid walls.

5. Conclusions

This study examined the behavior of a new two-fluid model for semidilute entangled polymer solutions in a pressure-driven channel flow. The thermodynamic model was based on the hypothesis that diffusional processes are responsible for the shear band formation in polymer solutions. An additional stress-diffusive term was used to control the smoothness and uniqueness of the profiles. The advantage of the new model is that the differential velocity was treated as a state variable, which simplified the specification of the slip boundary conditions. The computational results showed a plug-like profile of the velocity and concentration bands for the same range of pressure gradients. Increasing the value of the pressure gradient shifted the kink separating the shear bands to the center. The steady-state profile of the first normal stress difference monotonically increased from the center of the channel to a maximum value at the wall. The value of the nonlocal diffusivity constant did not significantly influence the total velocity and the wall shear stress. The polymer concentration showed the same temporal behavior for different values of the nonlocal diffusivity constant. However, the steady-state solution was more uniform when we used larger \(\tilde{D}_{nonloc}\). The results of the volumetric flow rate calculated using different values of the pressure gradient in the ramp-up and down tests agreed, thereby confirming the uniqueness of the solution. This profile showed a spurt at a critical pressure gradient, as experimentally observed in the pressure-driven shear flows of polymeric materials. We also studied the effect of wall slip using the linear Navier slip model to illustrate how to account for slip in our two-fluid framework.
that the slip velocity of the solvent had no significant effect on the solution, whereas changing the polymer slip vertically shifted the velocity profile. The study results as well as the simplicity of the model encourage us to analyze the model behavior in more complex flows, such as contraction. Furthermore, a systematic comparison with the experimental data is required to validate the hypothesis and predictions of the new model.

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Appendix A

The dimensionless forms of Eqs. (1)–(10) using the scalings introduced in Section 2 are as follows:

\[ E^{-1} \frac{\partial \tilde{v}}{\partial t} = -E^{-1} \tilde{v} \cdot \nabla \tilde{v} - \tilde{v} \beta + \tilde{v} \cdot \tilde{\sigma}, \]  

\[ E^{-1} \frac{\partial \tilde{\sigma}}{\partial t} = \frac{\chi}{\tilde{n}_p} \tilde{n}_p \tilde{v} + \tilde{v} \frac{\partial}{\partial t} \tilde{\sigma} - \varepsilon (\tilde{c} - I) \tilde{\sigma} + \tilde{D}_{\text{nonloc}} \tilde{\sigma}, \]  

\[ \sigma = \sigma_p (c - I) + \beta (\tilde{\nu} \tilde{v}^n + (\tilde{\nu} \tilde{v}^n)^T), \]  

\[ \tilde{\nu} = \tilde{\nu} + \frac{\chi}{\tilde{n}_p} \tilde{n}_p \tilde{\nu}_p. \]  

\[ \Delta \tilde{\nu} = \tilde{\nu} \cdot (\tilde{\nu} \tilde{\nu}_p), \]  

\[ \frac{\partial \tilde{n}_p}{\partial t} = \tilde{v} \cdot \tilde{\nu} \tilde{v} + \tilde{v} \cdot \tilde{\nu}_p + \tilde{v} \cdot \tilde{\nu}_p \tilde{\nu} + \tilde{v} \cdot \tilde{\nu}_p \tilde{\nu}_p \tilde{\nu}. \]  

\[ \tilde{n}_p = \tilde{n}_p (\tilde{c} - I) + \beta (\tilde{\nu} \tilde{v}^n + (\tilde{\nu} \tilde{v}^n)^T). \]
\[ \overline{\mathbf{v}} = \mathbf{v} - \frac{\mathbf{n}_p \cdot \Delta \mathbf{v}}{n_p + \chi_n} \cdot \Delta \mathbf{v}. \]  

(25)

References