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Prediction of excess pressure drop in contraction–expansion flow by molecular dynamics: Axisymmetric and planar configurations

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ABSTRACT

In this paper, non-equilibrium molecular dynamics is used to simulate the flow of a dilute solution of linear molecules (Boger fluid) and a simple fluid (Lennard-Jones) through axisymmetric and planar contraction–expansion geometries. The pressure flow condition is generated by adding an external force field F_e to the equation of motion for the velocity, which is coupled to Nose–Hoover dynamics to keep the temperature constant. According to the monomer-spring model of Kremer and Grest, linear molecules are represented; and the simple fluid consists of spherical particles, which interact by means of a Lennard-Jones potential. The rheological response of the fluids indicates that the Boger fluid and the simple fluid exhibit constant viscosity in the interval ($0.002 \leqslant \dot{\gamma} \leqslant 0.5$); additionally, the Boger fluid presents elastic effects under shear (first normal stress difference, N_1) which are quadratic at low shear rates. In pressure flow through the expansion–contraction, results indicate that when both fluids have the same viscosity, pressure profiles $P(x_1)$ in the axisymmetric geometry reveal a higher pressure drop (ΔP) in the Boger fluid, while in the planar geometry ΔP was the same for both fluids. Results also reveal that ΔP is closely related to the extensional strain rate ($\dot{\varepsilon}$) experienced by the fluid at the contraction entrance. The pressure drop is higher in the axisymmetric geometry because the change in the molecular conformation, as measured by the mean-square mass distribution tensor $\langle I_2^2 \rangle$, is 80% higher than in the planar case, resulting in an increase in the energy required to deform the molecule and the loss of mechanical energy. In the planar geometry, under the same extensional strain rate, the conformational change of the molecules in the Boger fluid at the contraction is then lower than in the axisymmetric geometry.

1. Introduction

This research work examines one of the benchmark problems in rheology, namely, the prediction of the excess pressure drop in the flow of non-Newtonian fluids through contraction–expansion geometries. Experimental studies show that polymer solutions of the Boger type exhibit a larger pressure drop than its Newtonian counterpart, both of the same viscosity, in axisymmetric but not in planar geometries. As discussed below, experimental evidence on the flow in micro-devices contraction–expansion suggests that at very high strain rates that are achieved in these devices, such excess pressure drop could also be observed in a planar configuration.

Nigen and Walters [1] performed experiments to reproduce the flow of two polymer solutions of constant viscosity, Boger fluid type, through axisymmetric and planar contractions; experiments were also replicated using Newtonian fluids with the same viscosity of the Boger fluid. In the axisymmetric configuration, results indicated that the Boger fluid exhibits larger pressure loss than the Newtonian fluid, and that this loss depends on the viscosity of the fluid and the vortex formation at the input of the contraction. Surprisingly, in the planar configuration, the Boger fluid exhibited the same pressure loss as the Newtonian liquid with absence of vortices at the input of the contraction. It is noteworthy that the experiments developed by Nigen and Walters [1] considered a wide range of contraction ratios ($2 \leqslant \hat{\beta} \leqslant 40$) and to achieve planar flow conditions in the rectangular configuration, the length of the contraction in the neutral direction L_3 was considerably larger than that in the flow direction L_1 and that of the gradient L_2. Finally, the authors conclude that the extensional strain rate is similar both in planar and in the axisymmetric configuration. A further study [2] confirms the relationship between the formation of vortices and excess pressure drop. In a work parallel to that of

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Nigen and Walters [1], Rothstein and McKinley [3] performed experiments to reproduce the flow of a solution of polystyrene Boger type through an axisymmetric expansion–contraction, with a contraction ratio of 4:1:4, where the Boger fluid and Newtonian viscosities were similar. Their results indicate the existence of an extra pressure drop in the Boger fluid above the one observed in the Newtonian liquid at the same flow rate, which increases monotonically with the Deborah number. They state that this extra pressure drop is associated with cycles of stress-conformation hysteresis and dissipation processes, such that the stress and end-to-end distance of the polymer molecules follow a path at the contraction entrance and they return to equilibrium through a different trajectory.

Apparently, the occurrence of hysteresis cycles and their relationship with viscous dissipation, as well as the extensional strain rate experienced by the fluid entering through the contraction are related to the existence of *epd* (excess pressure drop) in axisymmetric configurations. The existence of these hysteresis cycles has been experimentally and numerically predicted (at different length scales) [4–7]. Using non-equilibrium molecular dynamics, it has been established that in the flow of polymer solutions through the contraction–expansion geometries, the largest pressure loss occurs at the entrance of the contraction, and in this area of the flow domain a maximum in the viscous dissipation and extensional strain rate are revealed [7].

Apparently, the absence of the excess pressure drop in planar configurations is due to the low elastic response that the fluid exhibits in this geometry [2]. In this regard, it has been found that the extensional strain rate ($\dot{\varepsilon}$) experienced by the fluid depends on the geometry and contraction ratio ($\hat{\beta}$). In the axisymmetric geometry the extensional strain rate scales with the square of the contraction ratio ($\dot{\varepsilon} \approx \hat{\beta}^2$) while in the planar case the variation is linear ($\dot{\varepsilon} \approx \hat{\beta}$) [8–10]. Genieser et al. [11] states that the planar extensional flow through a slot induces a non-linear viscoelastic response of the fluid, and that this response cannot be substantially modified by changing the contraction ratio ($\hat{\beta}$). Recently, Castillo-Tejas et al. [7] simulated the flow of a solution of linear molecules and that of a single fluid, Lennard-Jones type, through an expansion–contraction planar configuration 2:1:2, using the molecular dynamics technique. The density of both fluids was chosen such that the fluids exhibit the same shear viscosity in the first Newtonian region of the flow curve (η versus $\dot{\gamma}$). It was found that the ratio Lc_1/Lc_2 (the length of the contraction in the flow direction (x_1) and in the gradient direction (x_2), respectively) affects substantially the pressure drop. When the ratio Lc_1/Lc_2 is equal to one, both fluids exhibit the same pressure drop, viscous dissipation and extensional strain rate; however, by increasing the ratio Lc_1/Lc_2 in the Boger fluid, larger pressure drops are predicted than those of the simple fluid (or Lennard-Jones fluid) with $Lc_1/Lc_2 = 1.0$. With values of the ratio Lc_1/Lc_2 larger than one, the Boger fluids experiences higher extensional strain rate and larger area of stress-conformation hysteresis. The strain rate ($\dot{\varepsilon}$) and hence the extensional stress are related to conformational changes of the fluid molecules through the contraction, and therefore, the molecular conformation along the flow path is different in axisymmetric and planar geometries.

The number of works using micro-devices to characterize and study the response of polymer solutions in extensional flow has increased. Recently, cross-slot micro-devices have been used to reproduce the extensional flow of diluted and semi-diluted solutions, obtaining information on stagnation points from measurements of pressure drop and birefringence [12–15]. Rodd et al. [16] used a 16:1 planar micro-contraction to study the flow field and the pressure drop of a polyethylene oxide solution, and found that there are significant extensional effects due to the very small length scales and to the associated high extensional strain. Additionally, the authors identified four flow regimes in the pressure drop measurements; elsewhere, similar conclusions were obtained [17,10,18–20].

Large extensional strain rates reached in micro-devices may enable elastic fluids to generate larger pressure drops than their Newtonian counterpart in planar geometries. Campo-Deaño et al. [21] reproduced the flow of a low viscosity Boger fluid through a planar hyperbolic micro-contraction (the fluids were prepared with aqueous polyacrylamide solutions of different concentrations to which sodium chloride is added). The rheological response of the solutions indicated that the addition of salt to the solution produces a viscosity decrease, such that at low concentrations the fluid exhibits a constant viscosity range similar to that of a Boger fluid. Results indicate that the pressure drop is larger in the Boger fluid than in the Newtonian liquid (water). However, it is important to note that the Boger fluid viscosity (aqueous solution of polyacrylamide) was larger than that of the Newtonian fluid (water), and that this difference in viscosity may be responsible for the larger pressure drop in the Boger fluid. The same issue should be considered in the pressure drop results of planar micro-contractions [16,22], and in previous works with molecular dynamics [6]. It is important to note that the *epd* reported by Nigen and Walters [1], and Rothstein and McKinley [3,8] in axisymmetric configurations considered that the viscosity of Boger fluid is similar to that of its Newtonian counterpart. In the present paper, predictions of the excess pressure drop are made taking care that the viscosity of the fluids in question is the same.

Presently, there are numerous numerical simulations at the continuum mechanics level oriented to predict the *epd*, as well as the number of constitutive equations used to reproduce the kinematics and dynamics of flow see [23–28]. In most works, shear thinning polymer solutions or Boger fluids are used, where predictions of the pressure drop are below the value exhibited by the Newtonian fluid (i.e., $epd < 1$). For example, Szabo et al. [23] use a FENE-CR model to simulate the flow of a Boger fluid through a 4:1:4 axisymmetric contraction–expansion. Their results indicate that at low Deborah numbers, the *epd* is less than one and depends on the extensibility parameter of the model (maximum extension of the polymer molecules). There are recent works [29,30] which state that the failure of the Oldroyd-B model in predicting the *epd* is associated with a strong dependence of the first normal stress difference N_1 respect to shear rate $\dot{\gamma}$ (quadratic for all shear rates). For axisymmetric configurations, it is shown that the prediction of *epd* depends on a balance between extensional viscosity η_E and N_1. The results are consistent with previous works establishing the importance of extensional stress in the flow through contraction geometries [31–34].

A review of experimental works and numerical studies reach the following conclusions: (1) when the viscosity of Newtonian and non-Newtonian fluid is similar, *epd* has been observed in axisymmetric but not in planar macro geometries; (2) *epd* is apparently related to the formation of vortices at the entrance of the contraction, hysteresis cycles, viscous dissipation and extensional strain rate; (3) the use of constitutive equations and continuous models has been partially successful in predicting the *epd*, and the success depends on a balance between the extensional viscosity (η_E) and the first normal stress difference (N_1); (4) and finally, an important issue is the extensional strain rate experienced by the fluid which again depends on the particular geometry. Based on the above conclusions, the objective of this work is to simulate the flow of two liquids (one Newtonian as a Lennard-Jones Fluid and a Boger fluid) of the same viscosity through contraction–expansion geometries both axisymmetric and planar. Simulations calculate the pressure field, velocity and molecular conformation along the central line of confinement. The analysis of these predictions aim to reveal important features on the origin of the *epd*.