Effect of Viscoelasticity on the Rotation of a Sphere in Shear Flow

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Abstract

When particles are dispersed in viscoelastic rather than Newtonian media, the hydrodynamics will be changed entailing differences in suspension rheology. The disturbance velocity profiles and stress distributions around the particle will depend on the viscoelastic material functions. Even in inertialess flows, changes in particle rotation and migration will occur. The problem of the rotation of a single spherical particle in simple shear flow in viscoelastic fluids was recently studied to understand the effects of changes in the rheological properties with both numerical simulations [D’Avino et al., J. Rheol. 52 (2008) 1331-1346] and
experiments [Snijkers et al., J. Rheol. 53 (2009) 459-480]. In the simulations, different constitutive models were used to demonstrate the effects of different rheological behavior. In the experiments, fluids with different constitutive properties were chosen. In both studies a slowing down of the rotation speed of the particles was found, when compared to the Newtonian case, as elasticity increases. Surprisingly, the extent of the slowing down of the rotation rate did not depend strongly on the details of the fluid rheology, but primarily on the *Weissenberg number defined as the* ratio between the first normal stress difference and the shear stress.

In the present work a quantitative comparison between the experimental results and the results from the simulations is made mainly by using a multimode Giesekus model with Newtonian solvent as constitutive model. The model is fitted to the experimentally obtained linear and nonlinear fluid properties and used to simulate the rotation of a torque-free sphere in a range of Weissenberg numbers similar to those in the experiments. A good agreement between the experimental and numerical results is obtained. The local torque distribution on the particle surface calculated by simulations is shown.

**Keywords:** Particle rotation, Viscoelasticity, Constitutive equations, Suspensions

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1. Introduction

This paper is part of a joint effort to elucidate the effect of the viscoelastic nature of the suspending medium on the slowing down of the rotation of a sphere in a viscoelastic fluid subjected to shear flow, as compared to the Newtonian case. This is a problem of fundamental importance in understanding suspension mechanics of particles in complex, viscoelastic fluids. The problem under investigation is the rotation of a single, non-Brownian sphere in bulk simple shear flow, under the assumptions of absence of inertia and gravity, and without slip of the fluid on the surface of the sphere. **With these assumptions, the rotational motion of the particle is governed by the so-called freely**
rotating condition, whereby the total torque acting on the particle must be zero. For a Newtonian fluid, under these conditions, the rotation speed of a particle $\omega$ (rad/s) is equal to half the vorticity and is given by the well-known equation \[3, 4, 5, 6\]:

$$\omega = \frac{\dot{\gamma}}{2}$$

with $\dot{\gamma}$ the average shear rate. The rotation speed of the particle is independent of the particle radius and viscosity of the fluid. As the flow-field around a particle is transient in nature in a Lagrangian sense (e.g. Happel and Brenner [7]), meaning that an individual fluid element goes through a complex and time-dependent deformation along its trajectory past the particle, rheologically complex fluids with time-dependent and nonlinear viscoelastic properties are expected to lead to differences in the velocity and pressure fields with respect to the Newtonian case.

Understanding the motion of individual particles should lead to a better insight in the structure and rheology of suspensions in viscoelastic media (see e.g. the recent review on trends in suspension rheology by Mewis and Wagner [8]). Moreover, the mechanism by which particles are dispersed in a complex fluid is determined by the torques and forces acting on them (actually, in force and torque-free particles it is the symmetric first moment and the disturbance velocity associated which play a key role), also making this apparently very fundamental topic of very practical relevance, as was pointed out by Astruc et al. [9]. These authors performed experiments on particle rotation at finite Weissenberg numbers and although the data were quite scattered, the trend showed that the particle rotation in viscoelastic fluids slows down when compared to the Newtonian case as elasticity increases. Qualitatively similar effects of slowing down of the particle rotation are also observed with increasing inertia, where the particle rotation rate slows down with increasing $Re$ [10, 11].

More detailed studies of the rotation of a single well defined particle in model
suspension fluids have recently been carried out by both numerical simulations and using experiments. D’Avino et al. [1] presented quantitative results from a full 3D computational study on the rotation of a spherical particle in a simple shear flow using different constitutive models: the Newtonian model as reference, the shear-thinning, purely viscous, inelastic Bird-Carreau model, the constant viscosity elastic upper-convected Maxwell model, the shear-thinning elastic Phan-Thien-Tanner model and the shear-thinning elastic Giesekus model. It should be pointed out that the parameters of the constitutive equations in [1] were not chosen to fit the rheology of experimental fluids. The study, indeed, aimed to evidence the influence of different non-linear properties (shear thinning, first and second normal stress differences) to the particle rotation rate. The steady-state and start-up rotation speeds, and streamlines around a particle were presented. It was found that, except for the Bird-Carreau and Newtonian models, where no elasticity nor time effects are present, all models resulted in a predicted slowing down of the rotation of the sphere, when compared to the Newtonian case. The sphere rotation rate was found to be slower as the Deborah number $De = \tau \dot{\gamma}$ (with $\tau$ the relaxation time) is larger. The slowest rotation rate was observed for the upper-convected Maxwell model. The effects of the viscoelasticity on the streamlines in the vorticity plane were also computed and showed that the fore-aft symmetry, characteristic of creeping flow, was broken due to the elasticity of the medium: the streamlines become tilted, the region of closed streamlines around the particle collapses and two zones appear with fluid back-flow as $De$ increased.

In Snijkers et al. [2], the same problem was studied experimentally using videomicroscopy in combination with a counterrotating plate-plate rheometer. A number of model suspending fluids, selected to highlight specific constitutive features, including a Newtonian liquid, a constant viscosity, highly elastic Boger fluid, a shear-thinning, broad spectrum viscoelastic polymer solution and a single relaxation time wormlike micellar surfactant solution were selected, prepared and characterized. Spherical particles of polystyrene and glass, in a size range
between 50 and 200 µm were dispersed in these fluids and their rotation was recorded and analyzed. It was shown that particle rotation slows down, when compared to the Newtonian case, when elasticity increases, in qualitative agreement with the findings in the simulations. For the Boger fluid, some transient results could be obtained which revealed a damped oscillatory response of the rotation speed. Despite the variation in constitutive properties and wide range of time scales of the fluids, it was found that the Weissenberg number, defined as
\[
Wi = \frac{N_1(\dot{\gamma})}{T_{12}(\dot{\gamma})}
\]
(with \(N_1\) the first normal stress difference and \(T_{12}\) the shear stress) sufficed to scale the steady-state data: the steady-state rotation speed rendered dimensionless by the shear rate of the spheres in the different fluids scales onto a single master curve as function of the Weissenberg number. This indicates that the slowing down in rotation finds its main origin in normal stress effects. A preliminary direct comparison between experiment and simulations using the single mode model results was carried out and the results compared favorably, giving a similar qualitative behavior. A quantitative agreement was not expected since, as remarked above, the rheological properties of the experimental fluids were not carefully described by the single-mode models considered in [1].

In this paper, we carry out a quantitative study between the experimental measurements reported in et al. [2] and novel numerical calculations by considering more realistic constitutive equations as compared to model fluids used in [1]. The rheological characterization of the experimental fluids used in Snijkers et al. [2] are fitted with a multimode Giesekus model with Newtonian solvent. Subsequently, these models are used in the simulations from D’Avino et al. [1] and a comparison between the experimentally obtained rotation speeds and the simulation results are made as function of the Weissenberg number. Furthermore, the simulation results are used to show the relevant local fields around the particle surface. The effect of fluid viscoelasticity on the local torque and pressure will be presented (the particle is freely rotating thus the total torque is zero but not the torque distribution). The effect of varying \(Wi\) for a given constitu-
tive model and the effect of the choice of the constitutive model at constant $W_i$ on torque distribution on the surface and on the rotation rate will be discussed.

2. Constitutive equations

2.1. The multimode Giesekus model with Newtonian solvent

In the present work, the multimode Giesekus model with Newtonian solvent is chosen as constitutive equation since it is fairly realistic, while being fairly simple at the same time. The Giesekus model [12, 13] is able to describe shear-thinning, variable normal stresses ($N_1$ as well as $N_2$), nonlinear time effects, an extensional viscosity with finite asymptotic values, non-exponential stress relaxation, and start-up curves with stress-overshoots using a single nonlinear parameter $\alpha$ together with the usual linear parameters (viscosity $\eta$ and relaxation time $\tau$). The nonlinear parameter $\alpha$ is called the mobility parameter and is associated with anisotropic Brownian motion and anisotropic hydrodynamic drag on a polymer molecule. Its value affects the degree of shear thinning of the model making it essentially “softer”.

The Giesekus model has been widely used with success to model wormlike micellar surfactant solutions [14], polymer solutions and melts [15, 16, 17] and has been used previously for fluid dynamics computer simulations [1, 17, 18, 19]. Superpositions of single mode Giesekus models can describe the shapes of experimentally measured material functions almost quantitatively [15]. The multimode Giesekus model with Newtonian solvent, along with its predictions in several rheological experiments, will be discussed here in some detail. The model can be written as:

$$T_E = 2\eta_S D + \sum_{k=1}^{n} T_{Pk}$$

with $T_E$ the extra stress tensor, $\eta_S$ the viscosity of the Newtonian solvent, $D = \frac{1}{2} ((\nabla v) + (\nabla v)^T)$ the rate-of-deformation tensor (with $v$ the velocity vector), $n$ the number of modes and $T_{Pk}$ the $k^{th}$ contribution to the extra stress tensor.
where can be calculated from:

\[
\tau_{Pk} \left( \frac{\partial}{\partial t} T_{Pk} + v \cdot \nabla T_{Pk} - (\nabla v)^T \cdot T_{Pk} - T_{Pk} \cdot (\nabla v) \right) + T_{Pk} + \frac{\alpha_{Pk} T_{Pk}^2}{\eta_{Pk}} = 2\eta_{Pk} D
\]

with \(\tau_{Pk}\) the \(k\)th relaxation time, \(\eta_{Pk}\) the \(k\)th partial viscosity, and \(\alpha_{Pk}\) the \(k\)th anisotropy parameter.

For small-amplitude (or linear) deformations, the Giesekus model simplifies to the predictions of the Upper-Convected Maxwell (Eqs. (2) and (3) with \(\eta_S = 0\) and \(\alpha = 0\)) or Jeffreys model (Eqs. (2) and (3) with \(\alpha = 0\)) [15]:

\[
G'(\omega) = \sum_{k=1}^{n} \eta_{Pk} \tau_{Pk} \omega^2 \quad \text{and} \quad G''(\omega) = \eta_S \omega + \sum_{k=1}^{n} \frac{\eta_{Pk} \omega}{1 + (\tau_{Pk} \omega)^2}
\]

with \(G'\) and \(G''\) the linear storage and loss modulus respectively, and \(\omega\) the frequency of the applied oscillation. To compare with experiments, the relaxation times and associated viscosities need to be determined.

The predictions for steady-state shear flow for the Giesekus model, as derived by Giesekus [12], are:

\[
\eta(\dot{\gamma}) = \eta_S + \sum_{k=1}^{n} \frac{T_{12k}(\dot{\gamma})}{\dot{\gamma}} = \eta_S + \sum_{k=1}^{n} \frac{\eta_{Pk}(1 - f_k)^2}{1 + (1 - 2\alpha_{Pk})f_k}
\]

for the viscosity,

\[
\Psi_1(\dot{\gamma}) = \sum_{k=1}^{n} \frac{N_{1k}(\dot{\gamma})}{\dot{\gamma}^2} = \sum_{k=1}^{n} \frac{2\eta_{Pk} \tau_{Pk} f_k (1 - \alpha_{Pk} f_k)}{\alpha_{Pk} (1 - f_k) (\tau_{Pk} \dot{\gamma})^2}
\]

for the first normal stress coefficient, and

\[
\Psi_2(\dot{\gamma}) = \sum_{k=1}^{n} \frac{N_{2k}(\dot{\gamma})}{\dot{\gamma}^2} = -\sum_{k=1}^{n} \frac{\eta_{Pk} \tau_{Pk} f_k}{(\tau_{Pk} \dot{\gamma})^2}
\]

for the second normal stress coefficient, with:

\[
f_k = \frac{1 - \chi_k}{1 + (1 - 2\alpha_{Pk}) \chi_k}
\]

and:
\[
\chi_k^2 = \frac{[1 + 16\alpha_{Pk}(1 - \alpha_{Pk})(\tau_{Pk}\dot{\gamma})^2]^{0.5} - 1}{8\alpha_{Pk}(1 - \alpha_{Pk})(\tau_{Pk}\dot{\gamma})^2}
\] (9)

Obtaining the \( \alpha_{Pk} \) from fitting the nonlinear data is not straightforward, especially when a specific fast relaxation mode is not contributing much to the nonlinear response. In this respect an important limit of the model, valid for each individual mode, is:

\[
\lim_{\dot{\gamma} \to 0} \frac{N_{2k}}{N_{1k}} = -\frac{\alpha_{Pk}}{2}
\] (10)

For most fluids this zero-shear ratio lies between \( \sim -0.6 \) and \( \sim 0 \) [20], providing a physical limit for \( \alpha_{Pk} \).

2.2. The single mode Oldroyd-B model

The Oldroyd-B model [21] has been used with some success to model the behavior of Boger fluids [22] as it predicts a steady shear viscosity and a first normal stress coefficient that are independent of shear rate. The single mode Oldroyd-B model can be written as:

\[
T_E = 2\eta_S D + T_P
\] (11)

with \( T_P \) the polymer contribution to the extra stress tensor which can be calculated from:

\[
\tau_P \left( \frac{\partial}{\partial t} T_P + \mathbf{v} \cdot \nabla T_P - (\nabla \mathbf{v})^T \cdot T_P - T_P \cdot (\nabla \mathbf{v}) \right) + T_P = 2\eta_P D
\] (12)

with \( \tau_P \) the polymer relaxation time and \( \eta_P \) the polymer viscosity. The predictions for steady-state shear flow for the single mode Oldroyd-B model [21] are a constant viscosity \( \eta = \eta_P + \eta_S \) and first normal stress coefficient \( \Psi_1 = 2\eta_P \tau_P \).

The second normal stress coefficient \( \Psi_2 \) is predicted to be zero.
3. Fitting the experimental rheological data

In this section, results are given for the fits of the multimode Giesekus model with Newtonian solvent to the rheological data of the different fluids for which extensive linear viscoelastic and nonlinear steady state data were reported in Snijkers et al. [2]. First some details of the fitting procedure are discussed, then the results of fitting the rheological data is presented for the three different fluids. A fitting of the flow curve of the Boger fluid with the simple Oldroyd-B model is also presented.

3.1. Fitting procedure

To fit the experimental data, the CONDOR algorithm from Vanden Berghen and Bersini [23] was used in a Matlab environment. The convergence of the algorithm was tested by changing the step sizes and the initial values over a wide range. The error function $F$ which is minimized is

$$ F = \sum_{i=1}^{m} \left( \frac{\text{exp} - \text{fit}}{\text{exp}} \right)^2 $$

(13)

with $m$ the number of experimental data points, ‘exp’ the experimentally measured values from the mastercurves and ‘fit’ the fitted values. A weighted error function was preferred over the Euclidean norm because of the wide range of the measured experimental data points. The weighted error function as defined in Eq. (13) equalizes the weight of data points with a low value and a high value. The number of relaxation modes was kept to a minimum, in order to minimize the computational effort. For the solvent viscosity $\eta_S$ an experimentally measured value is used when possible and as such, this value is not always used as a fitting parameter.

The linear data was used to fit the linear parameters $\tau_{P_k}$ and $\eta_{P_k}$, and, subsequently nonlinear data was used to determine the corresponding nonlinear parameters $\alpha_{P_k}$. This method was compared to the case where the linear and the nonlinear data were all fitted at the same time. Both methods were found to yield identical parameters to within 5%.
3.2. *The wormlike micellar solution (WMS)*

The WMS was chosen as a model fluid because its rheological behavior can be modeled with a single relaxation time [24]. The results of fitting the linear storage and loss modulus \(G'\) and \(G''\) with a single-mode Giesekus model are shown in figure 1a, the results for the steady-state nonlinear viscosity \(\eta\) and first normal stress coefficient \(\Psi_1\) are shown in figure 1b, along with the prediction of the second normal stress coefficients \(\Psi_2\). The values for the parameters which resulted from the fitting are summarized in Table 1. The zero-shear viscosity \(\eta_0\) in the Table is defined as \(\eta_0 = \eta_S + \eta_P\). Note that in figure 1b, the first normal stress coefficient is multiplied by 10 to ensure a clear presentation.

The solvent in the WMS fluid is ill-defined: it consists of water, some salts, and some free surfactant. Given the microstructure of the fluid and the chemical equilibrium in the solution, one cannot easily define the exact composition of the solvent and measure the solvent viscosity \(\eta_S\) directly. For the WMS, we choose to fit the solvent viscosity to the data and a value of 0.014 Pa·s was obtained (see Table 1). The solvent clearly contributes to the storage modulus \(G''\) at the highest frequencies (see figure 1a).

3.3. *The shear-thinning polymer solution (ST)*

The ST was chosen as a model fluid because it shows the multiple relaxation time characteristics of polydisperse polymer melts and concentrated solutions while having a fairly low viscosity at room temperature. The results of fitting the linear storage and loss modulus \(G'\) and \(G''\) with a four-mode Giesekus model are shown in figure 2a, the results for the steady-state nonlinear viscosity \(\eta\) and first normal stress coefficient \(\Psi_1\) are shown in figure 2b, along with the prediction for the second normal stress coefficient \(\Psi_2\). The values for the parameters which resulted from the fitting are summarized in Table 2. The zero-shear viscosity \(\eta_0\) is again defined as \(\eta_0 = \eta_S + \sum_{k=1}^{n} \eta_P k\). The solvent (Pristane) has a very low viscosity of 5.7 mPa·s when compared to the total zero-shear viscosity 78.8 Pa·s of the solution, and, as such, solvent contributions to the flow behavior of the solution can be neglected.
Four relaxation times were found to be the minimal number necessary to fit the data quantitatively well (see figure 2a), up to frequencies of 60 rad/s. Shorter relaxation times were not used because in the experiments on particle rotation these fast processes are not probed. One should also note in Table 2 that the values obtained from the fit for the nonlinear parameters $\alpha_{P3}$ and $\alpha_{P4}$ are too high to be realistic (see equation 10) and these values were set to 0.6 which results in only a slight deviation on the viscosity curve at the highest shear rates (> 40 s$^{-1}$), hence corresponding to a regime where rotation speed measurements were not performed.

3.4. The Boger fluid (BF)

The BF was chosen as a model fluid because it has a constant viscosity combined with a high elasticity. However, fitting the rheological data with a nonlinear model is quite challenging see e.g. Quinzani et al. [25]. The solvent (Infineum S1054) has a viscosity of 28.0 Pa·s at 25.1 °C. When comparing the solvent viscosity to the zero-shear viscosity of the solution (49.0 Pa·s), one can appreciate the dominant contribution of the solvent to the viscosity of the solution. It was verified that the preparation procedure of the BF did not affect the medium viscosity [26]. The measured value for the solvent viscosity $\eta_S$ has been used, and all the other model parameters are fitted.

A Giesekus model with a single mode was found to be sufficient to give a good description for the nonlinear viscosity and normal stress data. This is shown in figure 3b where the model predictions are reported with a dashed line. At relatively high rates, the steady flow behavior is well predicted. However, this is not the case for the limiting zero-shear $\Psi_1$ compared to the limit given by the linear data in the terminal region ($\sim$500 Pa·s$^2$).

As the rotation rate of a particle has been investigated in the low shear rate range as well, a dual mode Giesekus model was fitted to the whole set of data for the nonlinear steady state properties together with the limiting first normal stress coefficient $\Psi_{1,0}$ obtained from the the terminal region of linear viscoelasticity. The results for the dual mode Giesekus model for the steady flow

11
data are shown in figure 3b (solid line) and for the linear oscillatory data in figure 3a (solid line). Although the predictions for the first normal stress coefficient with the dual mode model are good in the whole shear rate range, the linear viscoelastic properties are ill-described, except at the lowest frequencies (figure 3a). The prediction for the first normal stress coefficient is approximately equal to the predictions of the single mode Giesekus at rates above 0.3 s$^{-1}$. In the same figure, the second normal stress coefficient is reported as well. Increasing the number of relaxation times gave a better fit to the linear viscoelastic data, but made the description of the normal stress differences as a function of shear rate worse.

Finally, a single mode Oldroyd-B model is used for the BF. This simple model is useful for the BF because it predicts a constant viscosity and a constant first normal stress coefficient in steady shear flow, a behavior which is approximately observed for the BF. The viscosity varies by about 10% over the measured shear rate range (figure 3b). The first normal stress coefficient, as found in steady flow experiments, is approximately constant as well (200 Pa·s$^2$), although the zero-shear value for this coefficient, from linear viscoelastic data is found to be higher (∼500 Pa·s$^2$). In figure 3b, the resulting predictions for steady flow are shown (dotted lines).

3.5. Comparison between the different fluids

In order to compare the particle rotation rate for the different fluids, it is useful to calculate a dimensionless elasticity parameter for each fluid. Here, following [2], the Weissenberg number $Wi$, defined as the ratio between the first normal stress difference and the shear stress, is chosen as measure for elastic versus viscous forces in a viscoelastic medium. In figure 4, the Weissenberg number is plotted versus shear rate for the different fluids. For each fluid the experimentally obtained Weissenberg number from the master curves (figures 1b, 2b and 3b) are shown (symbols) along with the predictions of the different constitutive models (lines) previously discussed. When comparing the data of the different fluids at a certain rate one can conclude that the Boger fluid is the
most elastic, followed by the WMS and then the ST.

In calculating the rotation rate as function of Weissenberg number to compare the experimental results in the different fluids, the Weissenberg number is calculated from the fitted models instead of the “random, best-fit functions” used previously [2]. Whereas these two approaches yield similar results when the data are being interpolated, the constitutive models provide a more rational method of estimating the Weissenberg numbers when no first normal stress data is available. As final remark, for the BF, where different models are available for the calculation of \( Wi \), the dual mode Giesekus model was used since it captures the correct rheological trends in a wider shear rate range as compared with the single mode Giesekus and Oldroyd-B constitutive equations.

4. Numerical method

The simulations are carried out by solving the equations governing the dynamics of a viscoelastic fluid around a sphere, i.e. the momentum and continuity equations plus the constitutive model using a finite element method. A cubic domain is chosen with the spherical particle located at the center. The domains are chosen sufficiently large compared to the particle radius in order to minimize the effect of the boundary conditions of the particle dynamics. **A domain length 30 times larger than the particle radius suffices to assure negligible interactions with the boundary conditions.** A mesh with unstructured tetrahedral elements is adopted, with a higher density of elements close to the sphere, where larger gradients are expected. Due to the symmetry of the problem, only one quarter of the full domain is considered (for more details we refer to [1]).

The momentum and continuity equations are decoupled from the constitutive equation, and an implicit stress formulation is used. In this formulation the time-discretized constitutive equation is substituted into the momentum balance in order to obtain a Stokes like system. This allows to consider viscoelastic fluids without a Newtonian solvent contribution in the model, as the WMS
and ST of the present work. Finally, the **torque-free condition is imposed through constraints on the spherical surface, by means of Lagrange multipliers.** In this way, the rotation rate is included as an additional unknown in the equation system. Further details on the numerical procedure can be found in [19] for a single-mode model. The extension to multi-mode constitutive equations is straightforward since each mode is solved separately (due to the decoupling procedure mentioned above) and the contribution to the momentum balance of each mode is just an addition to coefficients of the Stokes-like system.

5. Results

5.1. Rotation rate

We first report in figure 5 the particle angular velocity versus the Debo- rah number for the three suspending liquids. The **Deborah number is, in general, defined as the imposed shear rate times the fluid relaxation time.** This is actually the definition used for the WMS and the BF fluids (for the latter the single-mode Giesekus model is chosen. Since a accurate description of the ST fluid requires a multi-mode model, we cannot univocally identify a relaxation time. Therefore, we defined an average relaxation time as \( \tau_P = \frac{\sum_{k=1}^n \tau_{P,k} \eta_{P,k}}{\sum_{k=1}^n \eta_{P,k}} \) and an average Deborah number as \( De = \dot{\gamma} \tau_P \). For the case of a single-mode model, the previous definition gives the usual Deborah number definition. The figure shows that at low \( De \) the Newtonian value is correctly measured and predicted, while as \( De \) increases the sphere slows down. The three liquids show a different trend at large \( De \) values. The agreement between experiments and simulations is clearly good for all the three liquids throughout the investigated range of shear rates.

As already shown in [2], all the experimental data collapse on a single mas- ter curve if plotted versus the Weissenberg number. In figure 6 a comparison between the numerical simulation and the experimental results is shown. Most experimental data was already reported in Snijkers *et al.* [2]. However, to ob-
tain the values of the Weissenberg numbers corresponding to the shear rates at which the rotation speed of a particle was measured, a different procedure was used, as explained in section 3.5. For the ST fluid this does not make much difference, the procedure using a constitutive model slightly extends the range of data points to lower Weissenberg numbers. For the WMS however, the Weissenberg numbers obtained using the Giesekus model are slightly higher than those obtained using the best fit function in Snijkers et al. [2]. For the BF the results are similar again, but in the Weissenberg number range 0.3 – 0.7 the data points are situated somewhat below the other data points. This is most probably an effect of the model fit and the extrapolation used to calculate \( W_i \).

In the steady-state rheological data of the BF, shown in figure 3b, a plateau is visible in the first normal stress difference \( \Psi_1 \) at shear rates from \( 0.4 – 1.5 \text{ s}^{-1} \). The zero-shear value, as obtained from oscillatory measurements, is however much higher. As such, when going from low to high shear rates, there has to be a downturn of the first normal stress difference at some point. One can see this downturn in figure 3b, and in the obtained fit it occurs mainly between rates from 0.02 up to 0.05 \text{ s}^{-1}. It is possible that actually this downturn occurs at higher rates. If this is the case, the rotation data points in figure 6, in the range of shear rates mentioned, would shift slightly to the right, making them possibly collapse with the other data points. Some individual steady-state measurement showed this downturn to be around 0.3 \text{ s}^{-1}, the measurements were however at the edge of sensitivity of the rheometer and did not have a good reproducibility [2].

For the ST fluid a very good agreement between experiments and simulations is found for the four-mode Giesekus model (parameters as in Table 2). For the WMS (parameters in Table 1) the agreement is also excellent. For the BF, the dual mode Giesekus model predictions (parameters in Table 3), are shown as a solid dark grey line in figure 6. One can see that the curve from the simulations is similar to the experimental data although the trend is still slightly different and yields an overprediction of the rotation speed. The even more simple single mode Giesekus model (parameters as in Table 3) resulted in
an identical prediction as the dual mode model (the dashed grey line overlaps the solid grey line) indicating that the zero-shear properties and the much higher zero-shear normal stress coefficient does not affect the particle rotation in our case. To get better predictions the solvent viscosity $\eta_S$ was fitted to the rheology data instead of using an experimental value, since the solvent viscosity $\eta_S$ in the fluid itself is not known but taken to be identical to the value of the pure solvent, which might be incorrect. Trying this with a single and dual mode Giesekus model yielded no substantial difference, the results were practically identical with the dark grey line in figure 6 discussed before.

To assess the effect of shear thinning, the Oldroyd-B model is simulated and the results are compared in figure 6 with the experiments and simulations for the Giesekus models as a dotted dark grey line. Although the model does not predict any shear-thinning and the elasticity is clearly overpredicted at higher rates and underpredicted at lower rates (figure 3b), the result for the rotation speed is similar to the results from the single and dual mode Giesekus models.

Finally, higher Weissenberg numbers were investigated using simulations to extend the range covered by experiments. The results for the simulated WMS and ST fluids now clearly show the occurrence of a plateau at $\omega \sim 0$. For the Boger fluid numerical difficulties arise when the Weissenberg number increases, mainly due to the large value for the longest relaxation time (1 – 2 orders of magnitude higher than the ST and WMS) combined with the very small $\alpha$ values. However, we expect that, since the experimental and numerical solvent viscosity is a consistent part of the total viscosity, by increasing the shear rates the viscous stresses eventually start to dominate over viscoelastic stresses (which will level off) and an increasing in the rotation speed towards the Newtonian value might be observed. This is, of course, not the case for the other two fluids where a Newtonian solvent can be considered absent. In conclusion, the fair scaling of the experimental and simulation results of the rotation rate versus $Wi$ confirm that the first normal stress difference plays a major role in controlling the rotation rate.
5.2. Local fields

In view of the quantitative agreement between data and predictions for all fluids considered, we now exploit the simulations to catch details not directly accessed in our experiments. The rotation rate of the particle follows from the zero torque condition, with the total torque on the sphere:

\[ \mathbf{M} = \int_S \mathbf{m} R \, dS \]  

where \( S \) is the surface of the sphere, \( R \) is the particle radius and \( \mathbf{m} \) is the local torque vector per unit area given by:

\[ \mathbf{m} = \mathbf{n} \times (\mathbf{T} \cdot \mathbf{n}) \]  

in which \( \mathbf{n} \) is the outwardly directed normal vector and \( \mathbf{T} \) is the total stress tensor \( \mathbf{T} = -p \mathbf{I} + \mathbf{T}_E \). Expanding the quantity in the integral we obtain:

\[ \mathbf{m} = \mathbf{n} \times (\mathbf{T} \cdot \mathbf{n}) = (t_2 n_3 - t_3 n_2) \mathbf{i} - (t_1 n_3 - t_3 n_1) \mathbf{j} + (t_1 n_2 - t_2 n_1) \mathbf{k} \]  

with \( \mathbf{t} = \mathbf{T} \cdot \mathbf{n} \) being the surface traction and \((\mathbf{i}, \mathbf{j}, \mathbf{k})\) being the unit vectors. Due to the symmetry of the problem the only components from \( \mathbf{m} \) that contribute to the total torque are the components in the third term \( m_3 \).

In figure 7 the local torque distribution \( m_3 \) on the particle surface is reported. Only one quarter of the full geometry is shown. The colors are interpolated from the nodal values obtained from the steady state solution of the governing equations. The flow goes from the right to the left of the figure and therefore the sphere rotates in a clockwise sense. The Newtonian case is shown in figure 7a whereas figures 7b-7d refer to calculations using the Giesekus model for the WMS suspending fluid (parameters in Table 1) at \( Wi = 0.15 \), \( Wi = 1.3 \) and \( Wi = 2.75 \), respectively. The symmetric situation of the Newtonian case breaks down as \( Wi \) increases. Indeed, the maximum torque shifts towards the aft of the sphere. Instead, the positions of the minima stay essentially unaltered.

The streamlines in the vorticity plane are plotted as well. The streamlines have been calculated by integrating the kinematic equations \( \dot{x} = \mathbf{v}(x) \) with
\( x(0) = x_0 \) where \( v(x) \) is the steady-state velocity field. An adaptive Runge-Kutta algorithm is used for integration.

The streamlines are fully symmetric for the Newtonian case. For the viscoelastic case, as already shown in [1], the closed orbits around the particle become more and more distorted with increasing \( W_i \), correspondingly losing the fore-aft symmetry.

To show the symmetry properties of the local torque better, figure 8 reports \( m_3 \) as function of \( \beta/\pi \), with \( \beta \) the angle over the circumference given by the intersection of the particle surface and the \( xy \)-plane. The angle \( \beta \) is 0 at the intersection of the negative \( x \)-axis with the sphere and increases in a clockwise sense.

Again, calculated data for the WMS fluid are shown. For \( W_i = 0 \), the torque achieves a maximum at \( \beta = \pi/2 \) and a minimum at \( \beta = 0 \) and \( \beta = \pi \). A similar situation is found at the lowest non-zero Weissenberg number. Here a roughly symmetric profile is still evident. By increasing \( W_i \), the symmetry is lost.

The effect of viscoelasticity on the pressure field is given in figure 9. The pressure field \( p \) is the isotropic part of the total stress tensor \( T = -pI + T_E \). The angle \( \beta \) is defined as in figure 8. The symbols are nodal point values taken from the simulations whereas the lines are interpolating functions used to smooth the numerical error. The ragged plot of the pressure at large \( W_i \) is due to numerical errors. The raggedness is not a result of an improper numerical scheme, but related to the unstructured mesh using tetrahedrons which gives non-smooth error distributions. Clearly this could be improved by a more refined mesh, but this will not change the overall result. For \( W_i = 0.0 \), the pressure achieves a maximum at \( \theta = \pi/4 \) and, because of symmetry at \( \theta = 5/4\pi \) and a minimum at \( \theta = 3/4\pi \) (and \( \theta = 7/4\pi \)). A similar situation is found for the WMS suspending fluid at the lowest Weissenberg number. Here a roughly symmetric profile is still evident although the maximum and minimum values of the pressure are larger as the shear rate is enhanced. By increasing \( W_i \), the symmetry is
lost and the point of zero pressure moves towards an angle $\theta > \pi/4$. Furthermore, the region at lower pressure reduces its area on the spherical surface whereas the region at higher pressure spreads out, covering a larger surface on the sphere. Such effects are more and more pronounced as the Weissenberg number is higher. Hence the high pressure zones shift to the ‘equatorial’ regions where the local shear rates, and hence the normal stress differences which are strong functions of $\dot{\gamma}$, are the highest. For a particle subjected to a shear flow in the viscoelastic case, the pressure field becomes dominated by the contribution of the normal stresses.

Figures 7 and 8 refer to a specific liquid (WMS) at different Weissenberg numbers. We now show the influence of the suspending fluid itself by considering the WMS and the BF fluid, described through parameters as in Table 1 and 3. Figure 10a compares the predictions for the local torque $m_3$ for $Wi = 2.75$ for the two fluids considered. The torque is nondimensionalized by using the external shear stress $T_{12,\text{ext}}$ as characteristic stress (notice that $m_3$ has the dimension of a stress). Rather surprisingly, the trends reported in this figure show that, in spite of the different nature of the two fluids, the local torque distributions look rather similar. The latter occurrence might be possibly related to the $Wi$ scaling of the (nondimensional) angular velocity reported in figure 6, because the particle angular velocity is implicitly related to the torque distribution through the torque-free condition $M = 0$. In the same figure, the contribution to torque of the solvent in the BF fluid is also shown (white triangles). The graph shows that the solvent contributes for the largest part to the total torque, as one would expect by looking at the viscosity values in Table 3. Finally, the trend is symmetric and, as expected, the elastic components are responsible for the shift of the minima and maxima values.

Such a scaling, however, does not hold for other quantities, as, for example, the local shear rate and the local normal traction $-p + T_{rr}$ on the particle surface. (The latter quantity was also considered in [11] for the Newtonian case.
at finite $Re$. As first pointed out by Joseph [27], shear thinning may lead to an enhancement of local shear rates, entailing an amplification of the normal stress effects. Figures 10b-c compare the results for the local shear rate, as expressed by $\sqrt{2D : D}$ and nondimensionalized by the imposed shear rate $\dot{\gamma}$, and the local normal traction (nondimensionalized by $T_{12,ext}$), in the shear plane. Notice that, in figure 10b, the larger local shear rate values for WMS are a consequence of the shear thinning as compared to the BF fluid. The data reported in the figure refer to the same macroscopic $Wi$ as in figure 10a ($Wi = 2.75$), but no quantitative agreement is found for the local shear rate and normal traction distributions pertaining to the two different suspending liquids.

6. Conclusions

A quantitative comparison between experiments and simulations on the effect of medium viscoelasticity on the rotational velocity of a sphere in simple shear flow has been carried out using a multimode Giesekus model with Newtonian solvent as constitutive model. The number of the modes as well as the parameters for each mode have been evaluated by fitting the linear and nonlinear (steady state) rheological data for each fluid. The experimental results for a shear thinning polymer solution and a wormlike micellar fluid agree with the numerical simulations. For the Boger fluid, where different fits are considered, the simulations predict a weaker dependence on the $Wi$ number. Within experimental accuracy, the rate of rotation, rendered dimensionless by the shear rate, $\omega/\dot{\gamma}$, scales on a master curve with the Weissenberg number, $Wi = N_1/T_{12}$, which has been attributed to effects of normal stresses [2].

As a fair quantitative agreement is established, the numerical simulations are exploited to study the local distribution of quantities which are relevant in the phenomenology under investigation, i.e. the local torque and the shear rate profiles. The distribution of the local torque and pressure obtained by simulations shows the symmetry breaking as the Weissenberg number increases. By comparing the local torque distribution
between the WMS and BF, at the same $Wi$, a similar profile is found, thus possibly confirming the scaling of the rotation rate with $Wi$. However, this is not the case for other quantities such as the local shear rate and normal traction at the particle surface.

7. Acknowledgements

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References


Table 1: The best-fit parameters of the single Giesekus model to the rheological data of the WMS.

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<th>$\alpha_{P_k}$ (-)</th>
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Table 2: The best-fit parameters of the four-mode Giesekus model to the rheological data of the ST.

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<th>( \eta_{Pk} ) (Pa·s)</th>
<th>( \alpha_{Pk} ) (-)</th>
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Table 3: The best-fit parameters of the single-mode, dual-mode Giesekus models and the single-mode Oldroyd-B model to the rheological data of the BF.

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Captions

**Figure 1.** Best-fit curves of the single-mode Giesekus model (solid lines) to the rheological data of the WMS (symbols): (a) fits to the linear viscoelastic oscillatory data and (b) fits to the steady-state flow data (viscosity and first normal stress coefficient), the predicted second normal stress coefficients are also shown. The first normal stress coefficient has been plotted offset by a factor of 10 for the clarity of presentation.

**Figure 2.** Best-fit curves of the four-mode Giesekus model (solid lines) to the rheological data of the ST (symbols): (a) fit to the linear viscoelastic oscillatory data and (b) fit to the steady-state flow data. The predicted second normal stress coefficient is also shown.

**Figure 3.** Best-fit curves of the single-mode (dashed line), dual-mode (solid line) Giesekus models and the Oldroyd-B model (dotted line) to the rheological data of the BF (symbols): (a) fits to the terminal region of linear oscillatory data for a dual-mode Giesekus model, (b) fit to the steady-state flow data. For the dual-mode Giesekus model, the predicted second normal stress coefficient is also shown.

**Figure 4.** Weissenberg number ($\dot{\gamma}$) as a function of the shear rate ($\gamma$) for the different fluids, calculated from the experimental data (symbols) and the different constitutive models (lines).

**Figure 5.** Comparison between the experimental (symbols) and numerical (lines) particle rotation rate as a function of the average Deborah number.

**Figure 6.** Comparison between the experimental (symbols) and numerical (lines) particle rotation rate as a function of the Weissenberg number.
Figure 7. Local torque [Pa] contribution over the particle surface. The figure a) refers to a Newtonian suspending fluid ($Wi = 0.0$) whereas the figures b)-d) refer to the WMS fluid for different Weissenberg numbers: b) $Wi = 0.15$ c) $Wi = 1.3$ d) $Wi = 2.75$. The streamlines on the vorticity plane are also reported.

Figure 8. Local torque profiles over the intersection between the sphere surface and the vorticity plane for a Newtonian and the WMS suspending fluids (at different $Wi$).

Figure 9. Pressure profiles over the intersection between the sphere surface and the vorticity plane for a Newtonian and the WMS suspending fluids (at different $Wi$). The symbols are the simulation data and the lines are interpolating functions.

Figure 10. Comparison of the (nondimensional) torque (a), local shear rate (b) and local normal traction (c) of the Giesekus model fit to the WMS fluid, which includes shear thinning and the fit to the BF, without shear thinning.
Figure 1:
Figure 2:
Figure 3:
Figure 4:
Figure 5:
Figure 7:
Figure 8:
Figure 9: