Simulation of adhesive material using a novel viscoelastic stress method

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ABSTRACT
In this paper a novel method is proposed, where a constitutive equation for the viscoelastic stress is solved in a Lagrangian frame of reference, and the full stress tensor is interpolated to the Eulerian fluid grid. The method is validated for a 2D flow past a confined cylinder and used to simulate the 3D multiphase flow of adhesive application.

INTRODUCTION

In industry the demands on environmentally friendly products and processes increase which in turn increase the focus on lightweight composite materials. Such materials often cannot be welded, and the use of adhesives is therefore an alternative joining method. This requires new production processes for which a thorough understanding is needed in order to optimize the productivity and ensure sufficient strength and quality of the joints. A key part in understanding the processes is the ability to simulate the flow of adhesive materials, which often have complex rheology and may be both viscoelastic and thixotropic. It is therefore not sufficient to describe its rheology with purely shear thinning models, e.g. the Carreau fluid model, since such models lack the ability to describe storage of energy and transient stress relaxation.

Viscoelastic fluid flows have been subject to research for quite some time, since many applications depend on their complex nature. Examples of linear models of viscoelasticity are the Upper-Covected Maxwell (UCM) model and the Oldroyd-B model.[4] Although such models are used to simulate viscoelastic flows in the literature, see for example,[7,9,10,14] a clear disadvantage is that the normal stresses may grow unbounded. A variety of more physical non-linear constitutive models exists. One example is the Giesekus model,[4] which is the UCM model with an additional quadratic term that prevents normal stresses from growing too large. The FENE (Finitely Extensible Non-linear Elasticity) models,[6] treat the polymer chains as non-linear dumbbells, i.e. two beads connected by a non-linear spring. The springs have a finite extensibility-limit such that the spring constant grows large when the limit is approached. The PTT model[3] was proposed in 1977 and has been widely used for simulating viscoelastic flows since. Instead of viewing polymers as dumbbells, the PTT model is instead derived from network theory by treating the material as a network of entangled polymers. For examples of applications see .[10,15,18]

A problem that can occur in simulations of viscoelastic flows is numerical instabilities arising even for moderate Weissenberg numbers. This is known as the High Weissenberg Number Problem (HWNP).[8] A solution to this problem was proposed by Fattal and Kupferman,[11,12] in which the constitutive equation is transformed into an equation for the logarithm of the conformation tensor. This transformation results in additive contribution to the rate of change, rather than multiplicative, and reduces the high stiffness of the constitutive equation.

IPS IBOFlow[1] is an in-house incompressible flow solver developed at the Fraunhofer-Chalmers Research Centre for Industrial Mathematics in Gothenburg, Sweden. It includes a conjugated heat transfer solver[20] and can simulate two phase flows with the Volume of Fluids (VOF) method, of which the latter has recently been employed to simulate the laydown of shear thinning materials, e.g. for seam sealing application[17,21] and adhesive laydown.[22]

In this paper the aim is to further develop the adhesive laydown simulations with an advanced viscoelastic rheology model, as this is necessary to correctly predict the adhesive flow. A novel method is used in which the viscoelastic stress tensor is obtained from solving the PTT constitutive equation on a Lagrangian discretization consisting of massless particles being convected by the fluid. By interpolating the stress tensor to the fluid grid it is then taken into account explicitly in the momentum equation. The model is validated with experimental data for the flow past a confined cylinder and then used in a two phase flow process simulation of adhesive application.

EQUATIONS

The incompressible viscoelastic fluid flow is governed by the momentum and continuity equations,

$$\rho\frac{\partial u_i}{\partial t}+\rho u_j\frac{\partial u_i}{\partial x_j}=-\frac{\partial p}{\partial x_i}+\frac{\partial}{\partial x_j}\sigma_{ij}+\rho g_i, \quad (1)$$

$$\frac{\partial u_j}{\partial x_j}=0, \quad (2)$$

where ρ is the fluid density, u_i is the velocity, p is the total pressure and g_i is the gravity. Here, σ_{ij} denotes the extra stress tensor,

$$\sigma_{ij}=2\mu S_{ij}+\tau_{ij}, \quad (3)$$

with μ being the viscosity of the solvent, i.e. of the Newtonian fluid surrounding the viscoelastic polymers, and S_{ij} is the strain rate tensor and τ_{ij} is the viscoelastic (polymeric) stress tensor.

In general, the material can have a relaxation spectrum, where the viscoelastic stress tensor is the sum of the modal viscoelastic stress tensors $\tau_{ij}^{(k)}$,[3]

$$\tau_{ij}=\sum_k \tau_{ij}^{(k)}. \quad (4)$$

The viscoelastic stresses can also be described in terms of the conformation tensor, c_{ij}, a symmetric and positive definite tensor related to the microstructural state of the material,[19]

$$c_{ij}=\frac{\lambda}{\eta_p}\left(\tau_{ij}-\delta_{ij}\right), \quad (5)$$

where λ is the relaxation time, η_p is the polymeric viscosity contribution and δ_{ij} is the unit tensor. The evolution of the viscoelastic stresses is described with a constitutive model. In this work the Phan-Thien-Tanner (PTT) model is used, which reads, in terms of the conformation tensor,[19]

$$\lambda\overset{\triangledown}{c}_{ij}=-Y(c_{ij}-\delta_{ij}), \quad (6)$$

where $\overset{\triangledown}{c}_{ij}$ is the upper-convected derivative

$$\overset{\triangledown}{c}_{ij}=\frac{Dc_{ij}}{Dt}-c_{ik}\frac{\partial u_j}{\partial x_k}-\frac{\partial u_i}{\partial x_k}c_{kj}, \quad (7)$$

with the material time derivative,

$$\frac{Dc_{ij}}{Dt}=\frac{\partial c_{ij}}{\partial t}+u_k\frac{\partial c_{ij}}{\partial x_k}. \quad (8)$$

Y is a relaxation function,

$$Y=1+\varepsilon(c_{kk}-\delta_{kk})=1+\varepsilon(c_{kk}-3), \quad (9)$$

where ε is a material constant related to the extensibility of the polymer network. When multiple relaxation modes are used, one constitutive equation is solved for each mode. Equation (9) also exists in an exponential form, but in this work only the linear form is used, because of its simplicity and since this is a common choice in literature. To prevent instabilities at high Weissenberg numbers, Equation (6) is transformed into an equation for the logarithm of the conformation tensor, $\Phi=\log\mathbf{c}$,

$$\frac{D\Phi}{Dt}-(\Omega\Phi-\Phi\Omega)-2\mathbf{B}=\frac{Y}{\lambda}\left(e^{-\Phi}-\mathbf{I}\right). \quad (10)$$

The tensor $\mathbf{B}$ is a traceless and symmetric volume-preserving deformation in the principal axis of $\mathbf{c}$ and Ω is a pure rotation. This is commonly known as the log-conformation representation. For details on this transformation the reader is referred to.[11,12]

NUMERICAL METHOD

The in-house flow solver IPS IBOFlow is used to simulate the viscoelastic fluid flow. It is an incompressible flow solver which uses a Cartesian octree grid that is automatically generated and adaptively refined. All boundary conditions on internal objects are imposed using the mirroring immersed boundary technique.[13,16] This makes the grid generation automatic, which in turn minimizes the preprocessing time. Another key advantage is that moving objects are efficiently handled. The Volume of Fluids (VOF) method with the CICSAM convective scheme is used to simulate two phase fluid-fluid flows.

Equation (10) is solved on a Lagrangian discretization which is being convected by the fluid. In each Lagrangian fluid element a local ODE system describes the evolution of viscoelastic stresses and convection of the element,

$$\begin{bmatrix} \dot{\mathbf{x}}(t) \\ \dot{\Phi}(t) \end{bmatrix} = \begin{bmatrix} \mathbf{u}(\mathbf{x},t) \\ F(\Phi(t),\mathbf{x}(\mathbf{t}),t) \end{bmatrix}. \tag{11}$$

Here $\mathbf{x}(t)$ is the position of the fluid element at time t, $\mathbf{u}(\mathbf{x},t)$ is the local fluid velocity at time t and F denotes the right-hand side of Equation (10). The quantities in the right hand side of Equation (11) that are stored in the Eulerian fluid grid are obtained through interpolation to the position $\mathbf{x}$. The system (11) is solved with the Sundials ODE solver library, Cvode,[2] after which the full viscoelastic stress tensor is interpolated to the cell centers of the fluid grid. The octree discretization of the fluid grid is then used to calculate its divergence which is included in the momentum equation (1) in the explicit part of the stress tensor, σ_{ij}. Special care is put into keeping the Lagrangian fluid elements evenly distributed in the viscoelastic domain by adding and redistributing them between simulation time steps if needed.

For the case of two phase flows, the Volume of Fluids (VOF) method is used. It is thus sufficient for the Lagrangian fluid elements only to exist in the viscoelastic phase. This makes the method highly suitable, in terms of computational efficiency, for multiphase flows where only a small part of the fluid domain is occupied by a viscoelastic phase.

RESULTS

The proposed method is validated by simulating the two-dimensional viscoelastic flow of a polyisobutylene solution past a confined cylinder. A sketch of the flow geometry is shown in Figure 1. The radius of the cylinder, R, is 0.002 m. At the left boundary an inlet velocity $U = 0.0424\,\mathrm{m/s}$ is prescribed and at the right boundary an outlet is placed. The remaining boundaries are treated as walls. The fluid enters at the inlet with all viscoelastic stresses set to zero. It is therefore ensured that the length of the channel is sufficient for the flow to develop upstream of the cylinder and again downstream of the cylinder before exiting through the outlet. A four-mode PTT model is used to describe the viscoelastic properties of the polyisobutylene solution. The parameters in the respective viscoelastic modes are listed in Table 1. To estimate the Deborah number of the flow the average relaxation time is calculated by weighting the modal relaxation times with the respective modal polymeric viscosities, which for the parameters used results in De ≈ 0.93, see Baaijens et al[5] for more details. A grid size of $\Delta x = \Delta y = 4R/60$ is used, and simulations with even higher resolution showed that the solution is grid convergent.

In Figure 2 the streamwise velocity and the first normal stress difference, $N_1 = \tau_{xx} - \tau_{yy}$, are

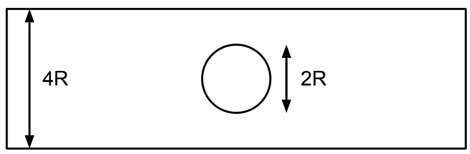

Figure 1. Symmetrically confined cylinder geometry.

Mode	η_p[Pas]	λ [s]	ε
1	0.443	0.00430	0.39
2	0.440	0.0370	0.39
3	0.0929	0.203	0.39
4	0.00170	3.00	0.39

Table 1. Parameters used in the PTT-model for the polyisobutylene solution.

shown along the channel centerline, whereas in Figure 3 they are shown across the channel at different locations. In both figures the simulation results are compared to experimental data obtained by Baaijens and colleagues.[5] The velocities have been normalized with the inlet velocity and the normal stress differences with the stress $\tau_0 = 62.179\,\text{Pa}$, in the same way as for the experimental data. An excellent agreement with the experiments is found for the velocity. The first normal stress difference also shows very good agreement throughout the flow, with a slight exception where it reaches its maximum at the stagnation point in the channel centerline just downstream of the cylinder. This is likely due to an underestimation of the strain rate in the interpolation to the Lagrangian fluid elements.

A flow where the cylinder is displaced one radius length in the vertical direction is also simulated. The inlet velocity is 0.0868 m/s, which corresponds to a Deborah number of 1.87. Again, the results are plotted and compared to experimental data obtained by Baaijens and colleagues,[5] along the channel centerline in Figure 4 and across the channel in Figure 5. Here the normal stress difference is normalized with the stress $\tau_0 = 127.291\,\text{Pa}$. For this flow an excellent agreement between simulation and experiments is found, both for the streamwise velocity and the first normal stress difference.

In summary, the results from the simulation of the flow past the confined cylinders show very good agreement with experimental data. This demonstrates that the simulation method is very promising in its ability to properly describe the physical characteristics of the viscoelastic flow.

Application of a highly viscoelastic adhesive is also simulated with the current simulation method. A single-mode PTT model is used and the two phase flow of adhesive and air is treated using the VOF method. The adhesive is injected into the fluid domain with velocity 0.48 m/s relative to the nozzle, which has diameter 2 mm and follows a linear path moving at 150 mm/s at constant distance 3.5 mm from the

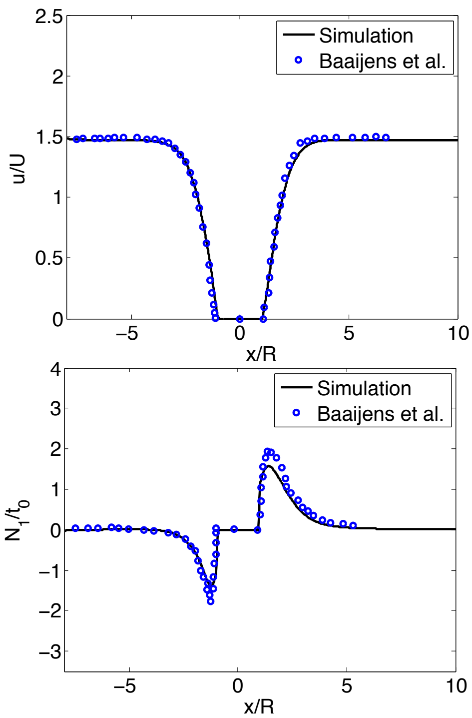

Figure 2. Streamwise velocity (top) and first normal stress difference (bottom) along the channel centerline for flow past the symmetrically confined cylinder.

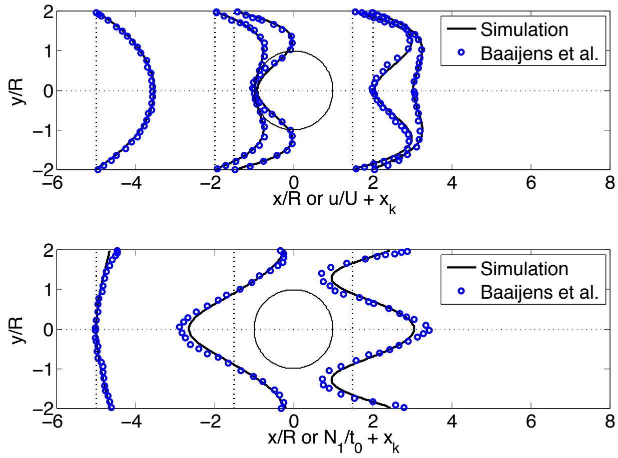

Figure 3. Streamwise velocity (top) and first normal stress difference (bottom) across the channel at different locations for flow past the symmetrically confined cylinder.

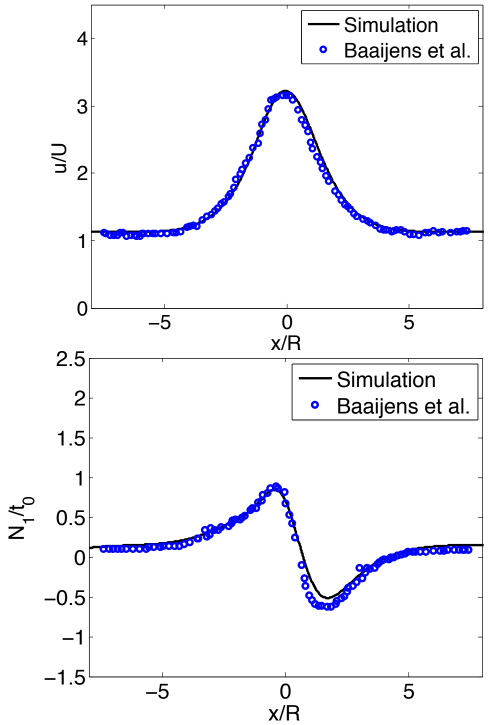

Figure 4. Streamwise velocity (top) and first normal stress difference (bottom) along the channel centerline for flow past the asymmetrically confined cylinder.

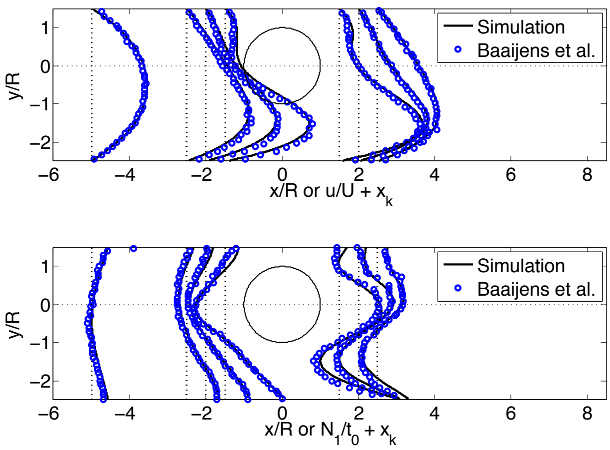

Figure 5. Streamwise velocity (top) and first normal stress difference (bottom) across the channel at different locations for flow past the asymmetrically confined cylinder.

bottom wall. The Reynolds number based on nozzle radius and injection velocity is 0.48 m/s and the Deborah number is 19.

The base grid consists of cubes with the side $\Delta x = 1\,\mathrm{cm}$ and in the simulations the grid is adaptively refined near the VOF-interface 5 and 6 times, respectively. This corresponds to finest cells being of size 0.32 mm and 0.16 mm, respectively.

In Figure 6 a snapshot from the finest simulation is shown. The Lagrangian grid is visualized as particles showing viscoelastic shear stress, and the Eulerian octree grid is shown in a cross-section plane. The Lagrangian fluid elements are distributed in such a way that there are always at least two fluid elements per fluid cell. Simulations with higher resolution show that the obtained solution is grid convergent.

To validate the simulations, a 3D-scan of a real adhesive bead applied by a robot-carried dispenser is used. The scanned bead is shown in Figure 7, where the two measurement positions used for cross section comparison are marked. In Figure 8 the simulated beads are compared in detail in the cross sections defined in Figure 7. Both simulations produce very good predictions of the height and width of the scanned bead. In addition, the finer simulation clearly predicts the convex shape of the bead near the three-phase contact between the air, the adhesive and the solid at the bottom wall. It should also be emphasized that surface tension has not been taken into account in these simu-

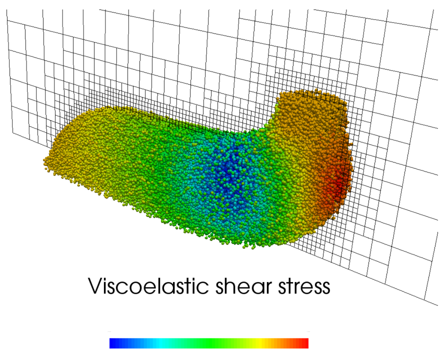

Figure 6. Viscoelastic shear stress in Lagrangian fluid elements.

lations, and the effect is thus fully contributed to viscoelasticity.

CONCLUSIONS

A novel method for simulation of viscoelastic flows was used to simulate the 2D flow past a confined cylinder and the 3D multiphase flow of adhesive application. In both cases the PTT constitutive model in the log-conformation representation was used to describe the evolution of the viscoelastic stresses. The results for the confined cylinder show that the method indeed predicts the characteristics of the viscoelastic flow both for a symmetrically and an asymmetrically positioned cylinder. Further, the adhesive laydown simulations produced beads that compared well with the scanned adhesive bead, thus demonstrating that the method at hand also is well capable of predicting the viscoelastic properties in two phase flow applications.

The results are very promising and a step towards accurate and efficient CFD simulations of industrial applications involving glues and adhesives, where the viscoelastic properties of the material are of great importance. A very important property of the current method is that the viscoelastic constitutive equation only needs to be discretized in the part of the domain occupied by viscoelastic material. For a two phase flow with only one viscoelastic phase, the computational effort is thus significantly reduced in comparison to a finite volume discretization for the 6 tensor components in the whole fluid domain. This, and the good resemblance of the experiments, show that the current method is highly suitable for such applications.

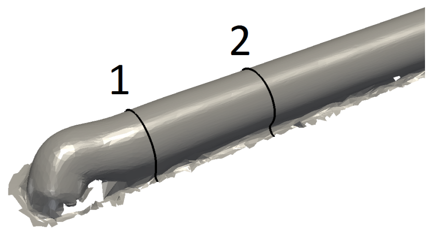

Figure 7. Scanned adhesive bead showing the two cross sections used for validation of the simulated beads.

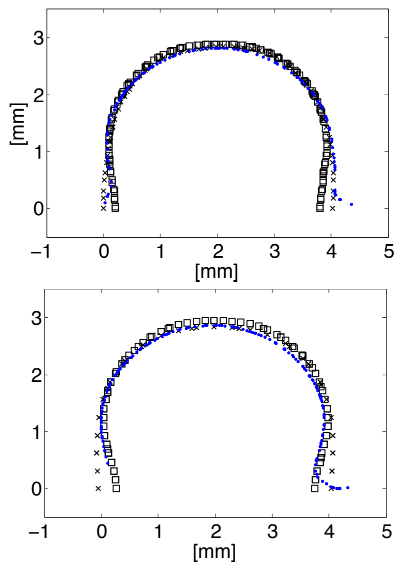

Figure 8. Cross section comparison at measurement position 1 (top) and 2 (bottom) between the bead simulated with 5 refinements (○), 6 refinements (□) and the scanned bead (●).

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