Validation of viscoelastic, non-isothermal fluid flow simulations

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ABSTRACT

The non-isothermal behavior of an Oldroyd-B fluid is modeled by temperature-dependent fluid properties via an Arrhenius approach and an internal energy balance that accounts for both energy and entropy elasticity. The numerical results for the temperature field in an axisymmetric 4:1 contraction flow with heated/cooled walls are compared to experimental data of a polyisobutylene based polymer solution (PIB-Boger fluid) and found to be in good agreement. Deviations are discussed.

INTRODUCTION

Large temperature gradients can frequently be encountered in polymer processing. This is due to the fact that heat transfer in these fluids is very low,[3] while the boundaries of the domain are often heated or cooled. In addition, viscous dissipation occurs locally, especially in the boundary layer where the velocity gradients are large, and leads to a local increase in temperature. Finally, the viscometric parameters are strongly dependent upon temperature and also influence the flow field.

Numerical flow simulations can contribute to a deeper understanding of the flow dynamics. To assure the correctness of the numerical approach, it is important to validate the used models by comparing the results to experimental data. For the current work, experimental data from Yesilata et al.[7] is used to investigate the validity of the suggested modeling approach. Yesilata et al. investigated a polyisobutylene based polymer solution (PIB-Boger fluid) in a circular 4:1 contraction flow with heated or cooled walls.

The Boger fluid was developed to close the gap between experimental observation and numerical prediction.[4] It shows nearly constant viscosity over a wide range of flow rates and its flow behavior can be modeled by a simple rate type model.[2] In the range of this work, the Oldroyd-B fluid model is employed. Non-isothermal behavior is simulated by allowing the model constants (viscosities and relaxation time) to vary with temperature.

For viscoelastic fluids, the 4:1 contraction flow is a popular benchmark test case. The geometrical singularity at the re-entrant corner is a challenge for the stability of the numerical approach, especially with increasing elasticity of the flow.

The paper is organized as follows: the thermorheological modeling is described in the next section, followed by a section describing the numerical setup and the test case. Afterwards, some key results are shown and discussed before the main points of the study are summarized.

THERMORHEOLOGICAL MODELING

The incompressible continuity and momentum balance equations describe the fluid dynamics. The viscoelastic fluid behavior is modeled by the Oldroyd-B fluid model. The stress tensor $\boldsymbol{\tau}$ is split into a solvent (Newtonian) stress tensor $\boldsymbol{\tau}_\mathrm{s}$ and the polymeric stress tensor $\boldsymbol{\tau}_\mathrm{p}$

$$\boldsymbol{\tau} = \boldsymbol{\tau}_\mathrm{s} + \boldsymbol{\tau}_\mathrm{p}. \tag{1}$$

The Oldroyd-B constitutive equation for the polymeric stress tensor is

$$\boldsymbol{\tau}_\mathrm{p} + \lambda \overset{\triangledown}{\boldsymbol{\tau}}_\mathrm{p} = 2\eta_\mathrm{p}\mathbf{D} \tag{2}$$

with the upper convected time derivative $\overset{\triangledown}{\boldsymbol{\tau}}_\mathrm{p}$ and the deformation rate tensor $\mathbf{D} = (\boldsymbol{\nabla}\mathbf{u} + (\boldsymbol{\nabla}\mathbf{u})^T)/2$. The non-isothermal behavior of the Oldroyd-B fluid is modeled by allowing the three model constants, solvent and polymeric viscosities η_s, η_p and relaxation time λ, to vary with temperature. An Arrhenius approach describes this dependence for the PIB-Boger fluid, the values of the constants are chosen according to the experimental data[7]

$$\frac{\eta_\mathrm{s}(T)}{\eta_\mathrm{s0}} = \frac{\eta_\mathrm{p}(T)}{\eta_\mathrm{p0}} = \frac{\lambda(T)}{\lambda_0} = a_\mathrm{T}(T). \tag{3}$$

Here $a_\mathrm{T}(T)$ is the Arrhenius shift factor, η_s0, η_p0 and λ_0 are the reference values of viscosities and relaxation time at reference temperature T_0. The shift factor is further dependent upon the activation energy ΔH and the universal gas constant R_u

$$a_\mathrm{T}(T) = exp\left[\frac{\Delta H}{R_\mathrm{u}}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right]. \tag{4}$$

The temperature field is calculated using the internal energy balance equation. Assuming the internal energy to depend solely upon temperature, it reads

$$\frac{\partial(\rho c_\mathrm{p} T)}{\partial t} + \mathbf{u}\cdot\boldsymbol{\nabla}\left(\rho c_\mathrm{p} T\right) - k\Delta T - Q = 0 \tag{5}$$

with density ρ, specific heat capacity c_p, velocity vector $\mathbf{u}$, thermal conductivity k and source term Q. The source term is assumed to include internal energy sources only. For viscoelastic fluids, these are composed of dissipative and elastic components. The ratio of these is locally dependent upon the flow characteristics,[8] but is simplified here by using a uniform splitting factor α for the whole fluid domain, following an approach of Peters and Baaijens.[5] Thus, the source term reads

$$Q = \boldsymbol{\tau}_\mathrm{s} : \mathbf{D} + \alpha\boldsymbol{\tau}_\mathrm{p} : \mathbf{D} + (1-\alpha)\frac{tr(\boldsymbol{\tau}_\mathrm{p})}{2\lambda(T)}. \tag{6}$$

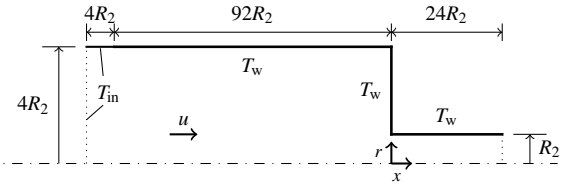

Figure 1. 2D sketch of the axisymmetric testcase geometry

TEST CASE SETUP

The foam-extend release of the OpenFOAM package[6] is used as basis for the implementation. It provides a Finite-Volume Method which is employed for the numerical discretization of the governing equations. The solution of the coupled set of balance and constitutive equations is achieved by a decoupled approach, based on the SIMPLE algorithm.[1] The stabilization library developed by Niethammer et al.[10] assured a stable solution of the constitutive equation of the polymeric stress tensor. More specifically, the root conformation representation first proposed by Balci et al.[9] is used for the presented results.

The shape of the fluid domain is sketched in Figure 1. An axisymmetric 4:1 contraction flow is investigated, the geometry is chosen equivalent to the experimental setup of Yesilata et al.[7] The radii of the two cylinders are $R_1 = 25.4\,\mathrm{mm}$ and $R_2 = 6.35\,\mathrm{mm}$. The inlet duct has a length of $96R_2$ in total, while the heating or cooling of the walls starts at $-92R_2$. The outlet duct has a length of $24R_2$.

At the inlet, a uniform velocity profile is imposed. In the experimental setup, the inlet is realized in form of a smaller tube of unknown diameter, so the velocity profile needs to develop in both setups. The inlet velocities at the respective Deborah numbers shown here are calculated from the Deborah and Reynolds-numbers given in the experiments. The temperature at the inlet and the first wall segment is imposed as 296.5 K, the reference room temperature of the experiments. For the stress tensor, a zero gradient is imposed at the inlet, allowing the stress profile to develop according to velocity and temperature profiles.

ρ	$880\,\mathrm{kg/m^3}$	c_p	$1970\,\mathrm{J/kg\,K}$
η_{s0}	$31\,\mathrm{Pa\,s}$	η_{p0}	$17\,\mathrm{Pa\,s}$
λ_0	$2.0\,\mathrm{s}$	T_0	$296.5\,\mathrm{K}$
k	$0.13\,\mathrm{W/m\,K}$	$\frac{\Delta H}{R_\mathrm{u}}$	$6414\,\mathrm{K}$

Table 1. Fluid properties

Grid	Control volumes	$\Delta x_{min}/R_2$
mesh 01	2060	0.096
mesh 02	6100	0.048
mesh 03	22520	0.024

Table 2. Mesh parameters

No-slip boundary conditions are employed for the velocity at the walls. The wall between $-96R_2$ and $-92R_2$ is given room temperature 296.5 K, all other walls are heated or cooled with respect to the inlet temperature.
At the outlet, a fixed pressure is assumed, all other field variables have a zero gradient boundary condition.
Fluid properties are presented in Table 1. Three different meshes, that are successively refined towards the singularity, are considered in order to investigate grid sensitivity. Table 2 indicates the mesh parameters.

RESULTS AND DISCUSSION

Three dimensionless numbers characterize the considered fluid behavior: the Reynolds number Re, the Weissenberg number Wi and the Deborah number De. While the Reynolds number describes the ratio of inertial to viscous forces $Re = \frac{\overline{u_{x,2}} R_2 \rho}{\eta_0}$, the Weissenberg number measures the ratio of elastic to viscous forces in a viscoelastic material $Wi = \frac{\lambda \overline{u_{x,2}}}{R_2}$, with the mean axial velocity in the outlet duct $\overline{u_{x,2}}$ and the total viscosity $\eta_0 = \eta_s + \eta_p$. The Deborah number is defined as the ratio of characteristic time of the fluid to the time scale of the process, yet it equals the Weissenberg number in the considered steady flow regime and both are treated equivalently here. The axial position of the measured data is denoted by the dimensionless axial coordinate $\zeta = x/R_2$. The origin of the coordinate system ($\zeta = 0$) is located at the contraction plane, so that values smaller than zero refer to the upstream section, values larger than zero to the downstream channel. The presented results are evaluated at an axial position $\zeta = -0.3$, slightly upstream of the contraction plane.

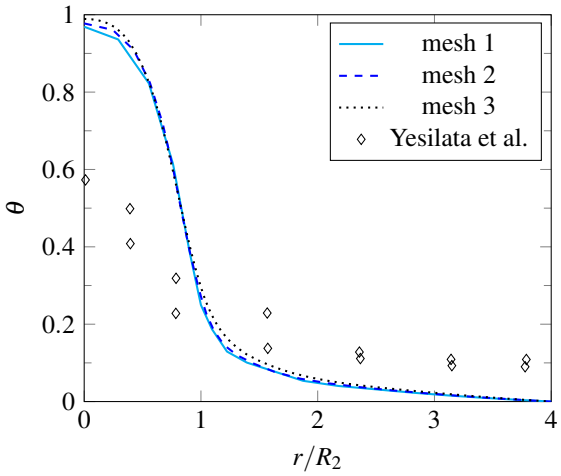

Figure 2. Non-dimensional temperature over radial position for a wall temperature of $T_\mathrm{w} = 285\,\mathrm{K}$ at $De = 5.04$

The temperature field data is non-dimensionalized as proposed by Yesilata et al.[7] in order to assure comparability. Reference values are the inlet temperature of the fluid $T_\mathrm{in} = 296.5\,\mathrm{K}$ and the wall temperature T_w of the considered test case, θ is the non-dimensional temperature $\theta = \frac{T_\mathrm{w} - T}{T_\mathrm{w} - T_\mathrm{in}}$.
Results are compared to the experimental data at two different wall temperatures: $T_\mathrm{w} = 285\,\mathrm{K}$ and $T_\mathrm{w} = 305\,\mathrm{K}$.

Figure 2 presents the non-dimensional temperature over the dimensionless radial coordinate at a wall temperature of 285 K and Deborah-number of $De = 5.04$. The results of the numerical simulations for three successively refined meshes are compared to experimental data reproduced from Yesilata et al.[7] The experimental data were measured from $r/R_2 = -4$ to $r/R_2 = 4$, both values are shown here in the positive radial coordinate. Although there are obvious deviations to the experimental data, the qualitative representation of the values is good. Deviations are most pronounced at the wall and at the centerline. At the radial coordinate $r/R_2 = 4$, the wall boundary condition would be expected. In

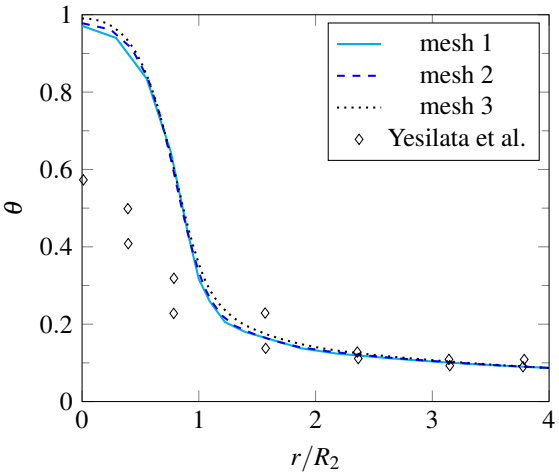

Figure 3. Non-dimensional temperature over radial position for a wall temperature of $T_w = 286\,\mathrm{K}$ at $De = 5.04$

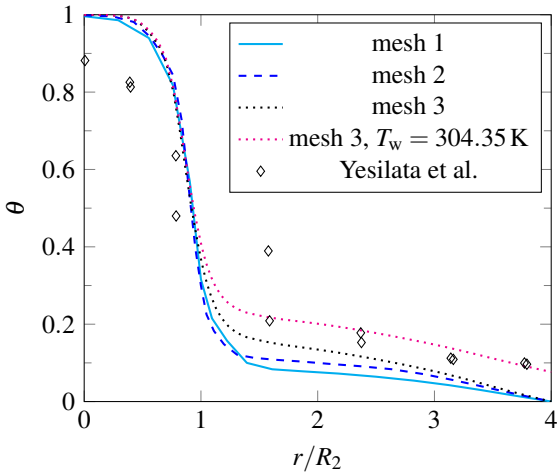

Figure 4. Non-dimensional temperature over radial position for a wall temperature of $T_w = 305\,\mathrm{K}/304.35\,\mathrm{K}$ at $De = 11.3$

the simulations, the nominal wall temperature, that is also used for non-dimensionalization of temperature is imposed. As expected, the simulation value for θ here is zero. The experimental data is not given at the wall, the temperature profile suggests however that θ is approximately 0.1 there, which would equal a wall temperature of about 286 K. What may have happened is that in the long test section, the wall temperature could not be kept entirely constant. In Figure 3 the radial temperature profiles for the three meshes of simulations at an imposed wall temperature of 286 K are presented. With this adjusted setup, the near-wall temperature profile of the experimental data can be reproduced almost exactly.

At radial position $r/R_2 = 0$, the deviation between experimental data and simulation data is more pronounced. Yet also this behavior could be expected of the numerical simulation. In the axisymmetric mesh geometry, the flow is almost two-dimensional. With the heat conduction being extremely low in polymeric solutions,[3] the only possibility for temperature to change in radial direction is heat production by viscous dissipation. Viscous dissipation occurs mainly where (pronounced) velocity gradients exist, that is at the wall and inside the re-circulation zone that forms in front of the contraction. In these regions, the temperature profile can be captured well. In the center of the tube, however, velocity gradients are small and consequently dissipation is small also. In the axisymmetric test case the flow symmetry in radial direction is enforced. The bulk temperature is only slightly reduced, while it is decreased significantly in the experimental data. Here however, the flow field is very unlikely to be fully symmetric. Disturbances can be expected to be encountered in any real flow, and are visualized here through the difference in the experimental data for the negative and positive radial segment. Disturbances create velocity gradients, and the dissipation is increased. In the experimental setup it is also possible that disturbances are imposed by the input of the temperature probes in the flow field. At this point it is important, to keep in mind the differences in the setup between numerical and experimental investigation. The numerical simulation shows the “perfect” flow conditions, that are most unlikely to occur for real flow. Keeping this in mind, the temperature profile can be reproduced in a satisfactory qualitative way.

Figure 4 shows the dimensionless temperature calculated on the three meshes for a heated wall of temperature $T_w = 305\,\mathrm{K}$ at a Deborah number of $De = 11.3$. The purple line represents the simulation on the finest mesh at an

imposed wall temperature of $T_w = 304.35\,K$ (which equals $\theta \approx 0.75$). The same effects can be seen as for the cooled wall. With the adjusted setup, the experimental data could be met in the vicinity of the wall. The bulk temperature is underpredicted, although the deviations to the experimental data are less pronounced than for the cooled wall. The deviation between the measured data points at the same radial position are also significant.

SUMMARY AND CONCLUSIONS

An approach for modeling the thermorheological behavior of an Oldroyd-B fluid is proposed and validated against experimental data of a polyisobutylene based polymer solution flow through a circular 4:1 contraction with heated or cooled walls.[7] The non-isothermal character of the Oldroyd-B fluid is realized by temperature-dependent model constants. These are related to reference values with an Arrhenius approach. The internal energy balance equation is derived following the work of Peters and Baaijens,[5] energy and entropy elasticity are included. Partitioning between both is achieved by defining an a priori splitting factor. In the numerical setup, an axisymmetric 4:1 contraction is investigated.

The results indicate that with the proposed model for the non-isothermal behavior of the considered viscoelastic fluid the temperature gradient near the wall can be well reproduced, while the bulk temperature tends to be underestimated for heated walls and overestimated for cooled walls, respectively. The deviations in the bulk temperature are assumed to be caused by the enhanced viscous dissipation in the experimental flow through disturbances in the flow field. These cannot be reproduced in the simulations, where a perfectly symmetric flow field is imposed by the axisymmetric test case setup.

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REFERENCES

1. Patankar, S. V. and Spalding, D. B. (1972), "Numerical prediction of three-dimensional flows", Imperial College of Science and Technology, Mechanical Engineering Department.

2. Boger, D. V. (1985), "Model polymer fluid systems", *Pure and Applied Chemistry*, **57**, 921–930.

3. Bird, R. B., Armstrong, R. C. and Hassager, O. (1987), "Dynamics of polymeric liquids. Vol. 1: Fluid mechanics", John Wiley and Sons Inc., New York, NY.

4. Boger, D. (1987), "Viscoelastic flows through contractions", *Annual Review of Fluid Mechanics*, **19**, 157–182.

5. Peters, G. W. and Baaijens, F. P. (1997), "Modelling of non-isothermal viscoelastic flows", *Journal of Non-Newtonian Fluid Mechanics*, **68**, 205–224.

6. Weller, H. G., Tabor, G., Jasak, H. and Fureby, C. (1998), "A tensorial approach to computational continuum mechanics using object-oriented techniques", *Computers in Physics*, **12**, 620–631.

7. Yesilata, B., Öztekin, A. and Neti, S. (2000), "Non-isothermal viscoelastic flow through an axisymmetric sudden contraction", *Journal of Non-Newtonian Fluid Mechanics*, **89**, 133-164.

8. Hütter, M., Luap, C. and Öttinger, H. C. (2009), "Energy elastic effects and the concept of temperature in flowing polymeric liquids", *Rheologica Acta*, **48**, 301–316.

9. Balci, N., Thomases, B., Renardy, M. and Doering, C. R. (2011), "Symmetric factorization of the conformation tensor in viscoelastic fluid models", *Journal of Non-Newtonian Fluid Mechanics*, **166**, 546–553.

10. Niethammer, M., Marschall, H., Kunkelmann, C. and Bothe, D. (2018), "A numerical stabilization framework for viscoelastic fluid flow using the finite volume method on general unstructured meshes", *International Journal for Numerical Methods in Fluids*, **86**, 131–166.