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Stress and strain amplification in a dilute suspension of spherical particles based on a Bird–Carreau model

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ABSTRACT

A numerical study of a dilute suspension based on a non-Newtonian matrix fluid and rigid spherical particles was performed. In particular, an elongational flow of a Bird–Carreau fluid around a sphere was simulated and numerical homogenization has been used to obtain the effective viscosity of the dilute suspension η^{hom} for different applied rates of deformation and different thinning exponents. In the Newtonian regime the well-known Einstein result for the viscosity of dilute suspension is obtained: $\eta^{hom} = (1 + [\eta]\varphi)\eta$ with the intrinsic viscosity $[\eta] = 2.5$. Here φ is the volume fraction of particles and η is the viscosity of the matrix fluid. However in the transition region from Newtonian to non-Newtonian behavior lower values of the intrinsic viscosity $[\eta]$ are obtained, which depend on both the applied rate of deformation and the thinning exponent. In the power-law regime of the Bird–Carreau model, i.e. at high deformation rates, it is found that the intrinsic viscosity $[\eta]$ depends only on the thinning exponent. Utilizing the simulation results a modification of the Bird–Carreau model for dilute suspensions with a non-Newtonian matrix fluid is proposed.

1. Introduction

In many applications polymers are filled with particles to improve usage properties of a final product. Those properties include: flame retardancy, UV resistance and mechanical properties (like Young's modulus). Yet often the filled polymer is processed in its molten state, thus the flow properties of the polymer–particle mixture are of great interest to the processing of the polymer and the final properties of the product. Filled polymers are very complex systems and have been a research topic for many decades. The complexity in describing those systems stems from a variety of interactions that particles can have with the surrounding polymer and with each other. In filled polymer systems it is, for example, observed that the particles influence the dynamics of the polymer chains close to their surface [1,2]. It is also not uncommon that filler particles build fractal agglomerates [1,3].

Since the seminal work of Einstein in 1906 [4,5] it is known that the viscosity of a liquid increases due to the presence of a small amount of spherical particles as:

$$\eta^{hom} = (1 + 2.5\varphi)\eta \qquad (1)$$

with η^{hom} the viscosity of the suspension, η the viscosity of the matrix fluid and φ the volume fraction of particles. Equation (1) holds in experiments up to approximately 3% volume fraction of particles [6,7]. Einstein's work was later extended by Batchelor and Green [8] to volume fractions of about 10%. For a Newtonian fluid filled with rigid spherical particles in a uniaxial extensional flow their result reads:

$$\eta^{hom} = (1 + 2.5\varphi + 7.6\varphi^2)\eta. \qquad (2)$$

All the aforementioned equations are derived for a Newtonian matrix. However, polymers are, in general, viscoelastic and often show non-linear (e.g. shear-thinning) behavior. Some authors have tried to apply the relations computed for a Newtonian matrix, e.g. (1) and (2), to non-Newtonian fluids. For that purpose one generally defines the so called hydrodynamic amplification factor:

$$X = \frac{\eta^{hom}}{\eta}, \qquad (3)$$

which is then used to amplify the resulting stress. Such a stress amplification approach has been proposed by Leonov [1]. Another approach – referred to as strain amplification approach – can be found in the work of Sarvestani and Jabbari [2], where the authors multiply the strain with the amplification factor X. In a recent paper [9] we proposed a different approach, named the stress and strain

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amplification approach (SSAA), where both the stress and the strain are amplified by different factors. One of those two factors is equal to the hydrodynamic amplification factor X and is used to amplify the stress similar to Leonov [1]. The second factor is referred to as the strain amplification factor a_d and defined by

$$\langle\dot{\boldsymbol{\gamma}}\rangle_m = a_d \dot{\boldsymbol{\gamma}}_0 \tag{4}$$

with $\dot{\boldsymbol{\gamma}}_0$ the applied rate-of-strain tensor and $\langle\dot{\boldsymbol{\gamma}}\rangle_m$ the rate-of-strain tensor averaged over the deformable volume in the suspension, i.e. over the matrix fluid. It can be shown that for arbitrary flows and matrix materials (viscous, elastic, viscoelastic) [4,8–10]

$$a_d = \frac{1}{1-\varphi}. \tag{5}$$

The factor a_d has been used in our previous study [9] to amplify the applied rate-of-strain tensor $\dot{\boldsymbol{\gamma}}_0$ in the non-linear constitutive models. Although such an approach brought a considerable improvement in the prediction of non-linear results compared with previously existing approaches, it fails to explain why the onset of shear thinning is observed at considerably lower shear rates as predicted by the value of a_d [11,12].

In this work only non-linear viscous effects are considered, hence viscoelastic properties of the polymer are ignored. For that purpose a generalized Newtonian fluid, specifically the Bird–Carreau model [13,14], is used to perform numerical simulations. The results of those simulations are used to obtain a better modification of non-linear constitutive models.

2. Modeling and simulation

The finite element method is used to perform computational fluid dynamics (CFD) where the Stokes equations are resolved with a non-linear viscosity function:

$$\begin{aligned} -\nabla p + \nabla\cdot\boldsymbol{\sigma} &= 0 \\ \nabla\cdot\boldsymbol{u} &= 0 \end{aligned} \tag{6}$$

Here p is the pressure, $\boldsymbol{\sigma}$ is the stress tensor and $\boldsymbol{u}$ is the velocity vector. A purely viscous matrix fluid which is described by a generalized Newtonian fluid model [13] is considered. In this case the stress tensor is defined as:

$$\boldsymbol{\sigma} = \eta(\dot{\gamma})\dot{\boldsymbol{\gamma}}, \tag{7}$$

where $\dot{\boldsymbol{\gamma}}$ is the traceless rate-of-strain tensor given by

$$\dot{\boldsymbol{\gamma}} = \nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^{\top}. \tag{8}$$

As follows from (7), an incompressible isotropic fluid is entirely characterized by one material parameter which is the non-Newtonian viscosity $\eta(\dot{\gamma})$. Therefore, further all results will be discussed in terms of $\eta(\dot{\gamma})$.

To describe the thinning effects in the steady-state viscosity $\eta(\dot{\gamma})$ of the matrix fluid the three-parameter Bird–Carreau model [14] is used

$$\eta(\dot{\gamma}) = \eta_0\left(1+(\lambda\dot{\gamma})^2\right)^{\frac{n}{2}}, \tag{9}$$

where η_0 is the viscosity of the matrix in the zero rate limit, λ is the characteristic time of the matrix and $n \leqslant 0$ is the thinning exponent. Further, $\dot{\gamma}$ in (7) and (9) is the effective deformation rate defined as

$$\dot{\gamma} = \sqrt{\frac{1}{2}\dot{\boldsymbol{\gamma}}:\dot{\boldsymbol{\gamma}}}. \tag{10}$$

We note that extreme thinning power-law behavior has been predicted and observed in the case of polymer melts (also filled), not only for a shear flow but also for an elongational flow [7,15].

The non-linear system of equations (6) is solved using a standard Galerkin finite element method [16,17]. The weak formulation of the problem is as follows:
find $(\boldsymbol{u}, p) \in \mathcal{W}$ such that

$$\begin{aligned} \int_\Omega \eta(\dot{\gamma})\,(\nabla\boldsymbol{u}:\nabla\boldsymbol{v})\mathrm{d}\Omega - \int_\Omega \nabla\cdot\boldsymbol{v}\,p\,\mathrm{d}\Omega = 0 \quad \forall\boldsymbol{v}\in\mathcal{V} \\ \int_\Omega q\,\nabla\cdot\boldsymbol{u}\,\mathrm{d}\Omega = 0 \quad \forall q\in\mathcal{Q} \end{aligned} \tag{11}$$

with $(\boldsymbol{v}, q) \in \mathcal{W}$ and $\mathcal{W} = \mathcal{V}\times\mathcal{Q}$, where $\mathcal{V}\in[H^1(\Omega)]^d$ and $\mathcal{Q}\in L^2(\Omega)$. $H^1(\Omega)$ is the Hilbert space and $L^2(\Omega)$ is the space of square integrable functions, $d = 3$ is the spatial dimension. A stable set of elements are the Taylor–Hood elements (P2P1) [18], the resulting non-linear system of equations is solved with a Newton–Raphson scheme using a direct solver.

The problem investigated in this study is in analogy to the original problem by Einstein [4,5], who considered a rigid sphere placed in the stagnation point of an elongational flow. The geometry of the representative volume element (RVE) is that of a cube with edge length $L = 1$ and a spherical hole at its center (at $\boldsymbol{x} = (0,0,0)^{\top}$), the radius of the sphere r being varied as 0.02, 0.03, 0.04, 0.05. The units of L and r are, in our case, arbitrary: they just have to be the same, e.g. both in meter or millimeter. The actual volume fraction of the particles is computed by a sum over the volumes of the elements in the mesh. Table 1 shows the computed volume fractions for the different radii used. The meshes used in the simulations are unstructured and graded towards the particle surface and have between ~12,000 and ~14,000 elements. Fig. 1 shows exemplary the mesh for the radius $r = 0.05$.

To reduce the computational effort the symmetry of the problem is taken into account and (6) is only resolved on one eighth of the geometry. Fig. 2 shows a sketch of the geometry and the boundary conditions used in this study. On the particle surface a no-slip condition, $\boldsymbol{u} = \boldsymbol{0}$, is applied. The velocity $\boldsymbol{u}_0$ is applied at the surface defined by $x = \frac{L}{2}$:

Table 1
Radii and the corresponding computed volume fractions of the particles.

r	φ
0.02	$3.32\cdot10^{-5}$
0.03	$1.13\cdot10^{-4}$
0.04	$2.67\cdot10^{-4}$
0.05	$5.23\cdot10^{-4}$

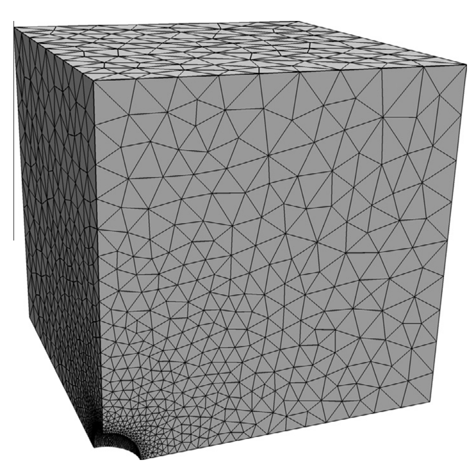

Fig. 1. Mesh used for the simulation for the particle with radius $r = 0.05$.