Introducing particles in viscoelastic fluids using a fluidity model

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Abstract

The complex dynamics of glass-forming liquids at a macroscopic level is characterized by non-linear (non-Newtonian) effects i.e. viscoelasticity and shear thinning, that depend on slow collective microstructural relaxation processes [1]. Different constitutive models can be used to describe the macroscopic behavior of these fluids, however, we use a phenomenological model to discuss the non-linear rheology by incorporating slow relaxation and flow induced rearrangements in the fluid. In our case we rely on a Maxwell-type constitutive equation to define the Eulerian stress ($\boldsymbol{\sigma}$) tensor appearing in the Navier-Stokes equations:

$$\overset{\triangledown}{\boldsymbol{\sigma}}(t) = G_\infty \boldsymbol{D}(t) - f(\vec{x},t)\boldsymbol{\sigma}(t), \tag{1}$$

We use the upper convected time derivative $\overset{\triangledown}{\boldsymbol{\sigma}}$ to account for the change of tensorial stresses due to flow advection. $\boldsymbol{D}$ and G_∞ are the symmetric shear-rate tensor and the low-frequency Maxwell plateau modulus, respectively.

We assume that the material's rheology is governed by a local relaxation rate $f(\vec{x},t)$, called fluidity [2, 3] which obeys a diffusion-relaxation equation:

$$\tau_f \dot{f}(\vec{x},t) = -\left(f(\vec{x},t) - \frac{1}{\tau_M(\dot{\gamma}(t))}\right) + D_f \nabla^2 f(\vec{x},t). \tag{2}$$

We include shear thinning effects through a steady-state relaxation rate as $1/\tau_M = 1/\tau + |\dot{\gamma}|/\gamma_c$, where $\dot{\gamma}$ is the local flow rate. This form captures the competition between the quiescent structural relaxation rate $1/\tau$ and flow-induced relaxation. Here, γ_c is a model parameter that signalizes the typical strain when local structures (nearest-neighbors cages in a fluid) break. Particularly heterogeneities in the flow could be accountable by using the diffusion term $D_f \nabla^2 f(\vec{x},t)$ in Eq. 2, then we can control how far fluidized regions could spread along their neighbors [3]. This model reproduces typical non-Newtonian flow effects of visco-plastic materials, e.g. plug flows in channels accompanied by shear banding, appearance of yield stress as $\tau \to \infty$, and pronounced memory effects.

In many biological and industrial processes particle-laden flows are encountered where mesoscopic particles are suspended in non-Newtonian fluids [4]. We study particle dynamics in such suspensions by describing the flow of viscoelastic fluids using Eqs. 1 and 2 combined with the Navier-Stokes equations, where the presence of external bodies, like particles, immersed in the fluid is included.

We specifically use a resolved method that combines Lagrangian Discrete Element Method (DEM) to track the bodies and Computational Fluid Dynamics (CFD) to solve the flow, introduced by [5]. The

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algorithm, called Fictious Domain Method (FDM), is a resolved method where particles or bodies have a large diameter with respect to the geometry they are immersed in, hence we can solve the flow around them by accounting for hydrodynamic forces exerted on the body and on the fluid, i.e. no drag models are used. The force exerted on the particles according to [6] consists of a pressure and a viscous term:

$$f = -\nabla p + \nabla \cdot \Sigma \tag{3}$$

$\nabla \cdot \Sigma$ represents the viscous forces coming from total stress in the flow $\Sigma = \boldsymbol{\sigma} + \nu \nabla \boldsymbol{u}$. Accordingly Σ includes both a Newtonian (where ν is Newtonian dynamic viscosity) and a non-Newtonian component, the latter defined by the constitutive equation 1.

The fully resolved simulation is implemented using immersed boundary conditions approach, in other words, the solid is considered a fluid with a constraint for the rigid component of motion and the fluid-solid interface condition is handled implicitly. The algorithm consists of the following steps [5, 6]: (a) the CFD calculation is carried out based on the constitutive equation for the fluid disregarding solid bodies, (b) the velocity information from the bodies is included and the force the fluid imposes on them is calculated, (c) correction of the velocity and pressure field, ensuring conservation equation, using the location and (angular) velocity of the bodies, where the latter depends on the force imposed by the fluid in equation 3. We use CFDEM@coupling and OpenFOAM and to perform all mentioned calculations.

Keywords: `particles, viscoelasticity, fluidity models, CFDEM, OpenFOAM, Shear thinning`

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