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Monolithic Newton-multigrid FEM for the simulation of thixotropic flow problems

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This contribution is concerned with the application of Finite Element Method (FEM) and Newton-Multigrid solvers to simulate thixotropic flows. The thixotropic stress dependent on material microstructure is incorporated via viscosity approach into generalized Navier-Stokes equations. The full system of equations is solved in a monolithic framework based on Newton-Multigrid FEM Solver. The developed solver is used to analyse the thixotropic viscoplastic flow problem in 4:1 contraction configuration.

1 Introduction

The thixotropy phenomena are introduced to yield stress material by taking into consideration the internal material micro-structure using a structure parameter. Firstly, the viscoplastic stress is modified to include the thixotropic stress dependent on the structure parameter

$$\begin{cases} \boldsymbol{\sigma} = 2\eta \mathbf{D}(\boldsymbol{u}) + \tau \dfrac{\mathbf{D}(\boldsymbol{u})}{\|\mathbf{D}(\boldsymbol{u})\|}, \text{ if } \|\mathbf{D}(\boldsymbol{u})\| \neq 0, \\ \qquad\qquad \|\boldsymbol{\sigma}\| \leq \tau, \text{ if } \|\mathbf{D}(\boldsymbol{u})\| = 0, \end{cases} \tag{1}$$

where $\mathbf{D}(\boldsymbol{u})$ denotes the strain rate tensor. The norm for a tensor Λ is given by $\|\Lambda\| = \sqrt{\mathrm{Tr}(\Lambda^2)}$. We use $\|\mathbf{D}(\boldsymbol{u})\|$ and $\|\mathbf{D}\|$ alternately. η denotes plastic viscosity, and τ defines a yield stress that is a threshold parameter from which the material starts yielding. The shear stress has two contributions: a viscous part, and a strain rate independent part. Secondly, an evolution equation for the structure parameter is introduced to induce the time-dependent process of competition between the destruction (breakdown) and the construction (buildup) inhabited in the material

$$\left(\frac{\partial}{\partial t} + u \cdot \nabla\right) \lambda = \mathcal{F} - \mathcal{G} \tag{2}$$

where, $\mathcal{F}$ and $\mathcal{G}$ are two nonlinear functions representing the buildup and breakdown of material micro-structure. A collection of thixotropic models with various choices of η, τ, $\mathcal{F}$ and $\mathcal{G}$ is given in Table 1;

Table 1: Thixotropic models

	η	τ	$\mathcal{F}$	$\mathcal{G}$
Worrall & Tulliani [1]	$\lambda\,\eta_0$	τ_0	$a(1-\lambda)\,\|\mathbf{D}\|$	$b\lambda\,\|\mathbf{D}\|$
Coussot et al. [4]	$\lambda^g\,\eta_0$		a	$b\lambda\,\|\mathbf{D}\|$
Houška [2]	$(\eta_0+\eta_1\lambda)\,\|\mathbf{D}\|^{n-1}$	$(\tau_0+\tau_1\lambda)$	$a(1-\lambda)$	$b\lambda^m\,\|\mathbf{D}\|$
Mujumbar et al. [5]	$(\eta_0+\eta_1\lambda)\,\|\mathbf{D}\|^{n-1}$	$\lambda^{g+1}G_0\Lambda_c$	$a(1-\lambda)$	$b\lambda\,\|\mathbf{D}\|$
Dullaert & Mewis [6]	$\lambda\eta_0$	$\lambda G_0(\lambda\,\|\mathbf{D}\|)\Lambda_c$	$(a_1+a_2\,\|\mathbf{D}\|)(1-\lambda)t^p$	$b\lambda\,\|\mathbf{D}\|\,t^{-p}$

where (η_0, τ_0) are initial plastic viscosity and yield stress in the absence of any thixotropic phenomena, (η_1, τ_1) are thixotropic plastic viscosity and yield stress. Λ_c is the critical elastic strain, and G_0 is the elastic modulus of unyielded material. a and b are buildup and breakage constants, and g, p, m, n are rate indices.

2 Quasi-Newtonian thixotropic flows models

In quasi-Newtonian modeling approach for thixotropic flows, an extended viscosity $\mu(\cdot,\cdot)$ is used for the generalized Navier-Stokes equations [8]. As for instance [3],

$$\mu(D_{\mathrm{II}}, \lambda) = \eta(D_{\mathrm{II}}, \lambda) + \tau(D_{\mathrm{II}}, \lambda)\frac{\sqrt{2}}{2}\frac{1}{\sqrt{D_{\mathrm{II}}}}\left(1 - e^{-k\sqrt{D_{\mathrm{II}}}}\right) \tag{3}$$

k is the regularization parameter. The generalized Navier-Stokes equations and the evolution equation for the structure parameter constitute the full set of modeling equations, which is given as follows

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$$\begin{cases} \left(\frac{\partial}{\partial t} + u \cdot \nabla\right) \boldsymbol{u} - \nabla \cdot \left(2\mu(D_{\mathrm{II}}, \lambda)\mathbf{D}(\boldsymbol{u})\right) + \nabla p = 0 & \text{in } \Omega \\ \nabla \cdot \boldsymbol{u} = 0 & \text{in } \Omega \\ \left(\frac{\partial}{\partial t} + u \cdot \nabla\right) \lambda - \mathcal{F}(D_{\mathrm{II}}, \lambda) + \mathcal{G}(D_{\mathrm{II}}, \lambda) = 0 & \text{in } \Omega \end{cases} \tag{4}$$

where $\boldsymbol{u}$ denotes velocity, p the pressure, λ the structure parameter, $\mathcal{F}$ and $\mathcal{G}$ the nonlinear functions for buildup and breakdown of material micro-structure. $D_{\mathrm{II}} = \frac{1}{2}\left(\mathbf{D}(\boldsymbol{u}) : \mathbf{D}(\boldsymbol{u})\right)$ is the second invariant of the strain rate tensor $\mathbf{D}(\boldsymbol{u})$.

3 Newton-Multigrid FEM Solver

The Newton-Multigrid FEM Solver is a monolithic approach for solving the full system of equations all at once. Firstly, we use a stable FEM approximation pair for velocity and pressure with biquadratic velocity and discontinuous pressure Q_2/P_1^{disc}, and biquadratic Q_2 for structure parameter with the appropriate stabilization for the convective terms. Secondly, the discrete nonlinear system is treated with generalized Newton's method w.r.t. the Jacobian's singularities having a global convergence property. Thirdly, the linearized systems inside the outer Newton loops are solved using a geometrical multigrid solver with a Vanka-like smoother. The combination of a stable finite element approximations, Q_2/P_1^{disc}, together with multigrid results in a high numerically accurate, flexible, and efficient FEM-multigrid solver. For details, we refer to [7].

4 Numerical Results

We investigate numerically Houška's [2] thixo-viscoplastic material in a 4:1 curved contraction configuration. The fully-developed flow conditions according to Houška thixotropic model are imposed at entry and exit together with no-slip on the top and bottom walls of reservoir and downstream channel. Our emphasis is to examine the transitions in shape and extent of the unyielded zones w.r.t breakdown parameter on isobands of material micro-structuring level λ. Figure 1 illustrates the impact of thixotropy breakdown parameter b. In fact, increasing the breakdown parameter induces more beakdown layers close to the walls of downstream channel, which prevent the material from rest inside long pipelines, typically used in transportation of waxy crude oils. In consequence, the design for the pipelines needs to be revisited taking in consideration the thixotropic phenomena inherited in the material. Furthermore, it is interesting to observe that unyielded zones in upstream

(i) Upstream channel & Entrance zone **(ii) Downstream channel**

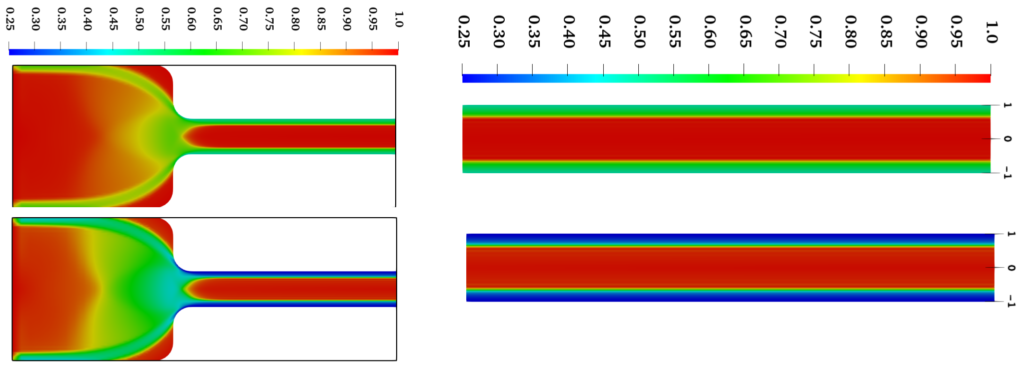

Fig. 1: Thixotropic flows in contractions: Impact of breakdown parameter b on λ isobands for thixotropic flows. While the other parameters are set to constants $\eta_0 = \eta_1 = 1.0$, $\tau_0 = 0.0$, $a = 1.0$,$\tau_1 = 2.0$, and $k = 10^4$.

and downstream parts of contraction domains do not merge at all. Physically, this happens because the unyielded material in the vicinity of center of reservoir becomes more rigid (or less flexible due to its inelastic nature). That means, the material can not deform elastically. Thus, when the material elements cross the contraction zone, they are not able to undergo even a small scale elastic crosswise extension, and thus remain disconnected and travel like a rigid-body in downstream channel. Further investigations are to consider the nonzero flow below the critical yield stress limit by considering the elastic behaviour in more general model i.e. thixotropic elasto-viscoplastic models.

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