Simulation Tests of the Constitutive Equation of a Nonlinear Viscoelastic Fluid

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Outline

• Rheometry of viscoelastic fluids
  • Measurements with a rotational rheometer
  • Motivations for FEM modeling

• Simulation of shear flow rheometry with COMSOL Multiphysics

• Results:
  • Normal force simulation
  • Rod climbing (Weissenberg effect) simulation
Rheometry of viscoelastic fluids

- Shear flow tests: non-Newtonian flow
- Small Amplitude Oscillation Shear (SAOS) tests: loss and storage modulus, linear properties
- Large Amplitude Oscillation Shear (LAOS) tests: anharmonic analysis, nonlinear viscoelastic properties
Rheometry of viscoelastic fluids

• Shear flow tests: non-Newtonian flow
• Small Amplitude Oscillation Shear (SAOS) tests: loss and storage modulus, linear properties
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Rheometry of viscoelastic fluids

- Angular Frequency (1/s)
- Storage and Loss Moduli (Pa)
  - G' at 60 °C
  - G'' at 60 °C
  - G' to 60 °C from 120 °C
  - G'' to 60 °C from 120 °C
  - G' to 60 °C from 0 °C
  - G'' to 60 °C from 0 °C

- Viscosity (Pa s)
  - Computed Steady Shear Viscosity
  - Measured Steady Shear Viscosity
  - Measured Complex Viscosity
  - Computed Steady Shear Viscosity WM
  - Computed Complex Viscosity WM

Angular Frequency, Shear Rate (1/s)

Storage and Loss Moduli (Pa)
Rheometry of viscoelastic fluids

- Silicone oil, (Polydimethylsiloxane, PDMS)
- High viscosity: 100 – 2000 Pa*s
- Viscoelastic fluid: 3 – 5 Maxwell elements for lumped parameters models
- Shear thinning, Cox-Merz rule, Nonlinear viscoelasticity
- Normal force measurements with CP geometry, Weissenberg-effect
Rheometry of viscoelastic fluids

Weissenberg effect:
Rheometry of viscoelastic fluids

Weissenberg effect:
Rheometry of viscoelastic fluids

Weissenberg effect:
Motivations for a FEM simulation

• Which 3D constitutive equation (e.g. UCM, Jeffreys, White-Metzner, Oldroyd, ...) is the best to model the fluid?

• How much is the effect of rod climbing on the measured viscosity?
Simulation of shear flow with COMSOL

CP-model: Cone-Plate (CP)

CC-model: Concentric Cylinder (CC)
Simulation of shear flow with COMSOL

- Swirl flow with two phases: silicone oil and air, surface tension and gravity included ->
  
  **2D axial sym., level set**

- Silicone oil: White-Metzner with 3 elements ->
  
  **2D PDE modes (cyl. coo.)**
Simulation of shear flow with COMSOL

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  2D PDE modes (cyl. coo.)

\[ \rho \frac{\partial \mathbf{u}}{\partial t} + \rho (\mathbf{u} \nabla) \mathbf{u} = \nabla [-p \mathbf{I} + \mathbf{\tau}] + \mathbf{F} \]

\[ \mathbf{\tau} = \sum_{j=1}^{n} \mathbf{\tau}_j \]

\[ \mathbf{\tau}_j + \frac{\eta_j (| \dot{\gamma} |) \nabla}{k_j} \mathbf{\tau}_j = -\eta_j (| \dot{\gamma} |) \cdot \left[ \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right] \]

\[ \nabla \mathbf{\tau}_j \equiv \frac{\partial \mathbf{\tau}_j}{\partial t} + (\mathbf{u} \nabla) \mathbf{\tau}_j - \left[ \mathbf{\tau}_j (\nabla \mathbf{u}) + (\nabla \mathbf{u})^T \mathbf{\tau}_j \right] \]
Simulation of shear flow with COMSOL

- Boundary conditions
- Variable scalings
- Time dependent solution, initialization
- Ramping up the azimuthal velocity
- Ramping up the coupling (Volume Force)
- Many variables, large RAM
Simulation of shear flow with COMSOL

- Reference simulation: Newtonian fluid, torque
Results – CP

CP-model:

Cone-Plate (CP)
Results – CP: Normal force

- Pressure distribution on the upper (conical) surface
Results – CP: Normal force
Results – CC

CC-model:

Concentric Cylinder (CC)
Results – CC: Rod climbing
Results – CC: Rod climbing
Results – CC: Torque, viscosity
Conclusions

• COMSOL is able to give the solution of this difficult problem
• Normal force values from CP simulation are in good agreement with measurements
• Rod-climbing in CC simulation is close to reality, computed changes in torque values mostly cancel, therefore viscosity measurements are not disturbed

Thank you for your attention!