International Day of Women and Girls in Science

Heat transfer processes using viscoelastic fluids in laminar and turbulent regimes

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Introduction: Viscoelasticity

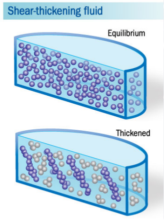
What is viscoelasticity?

- Fluids depending on their behaviour under the action of shear stress, can be classified as Newtonian and non-Newtonian.
- Viscoelastic fluids are a specific type of non-Newtonian fluids that exhibits a combination of elastic and viscous effects.
  - Visco: friction, irreversibility, loss of memory.
  - Elastic: recoil, internal energy storage.
- They have "memory": the state-of-stress depends on the flow history.

Introduction: Viscoelasticity

Other industry applications

- Most viscoelastic fluids are made of, or contain polymers (polymer solutions and polymer melts).



Introduction: Modelling of polymeric fluids

Like all fluids, viscoelastic fluids are governed by:

- Momentum equation: $\rho \frac{\partial \boldsymbol{u}}{\partial t} + \rho \boldsymbol{u} \cdot \nabla \boldsymbol{u} - \nabla \cdot \mathbf{T} + \nabla p = \boldsymbol{f}$
- Continuity equation: $\nabla \cdot \boldsymbol{u} = 0$

For Newtonian viscous fluids:
$\mathbf{T} = \eta(\nabla \boldsymbol{u} + \nabla^t \boldsymbol{u})$

For Polymeric fluids:
$\mathbf{T} = \eta_s(\nabla \boldsymbol{u} + \nabla^t \boldsymbol{u}) + \boldsymbol{\sigma}$

Introduction: Constitutive models.

$$\rho\frac{\partial \boldsymbol{u}}{\partial t} + \rho\boldsymbol{u}\cdot\nabla\boldsymbol{u} - \nabla\cdot\mathbf{T} + \nabla p = \boldsymbol{f} \text{ in } \Omega, t \in]0, t_f[,$$

$$\nabla\cdot\boldsymbol{u} = 0 \text{ in } \Omega, t \in]0, t_f[,$$

$$\frac{\lambda}{2\eta_0}\frac{\partial\boldsymbol{\sigma}}{\partial t} - (1-\beta)\nabla^s\boldsymbol{u} + \frac{\lambda}{2\eta_0}\left(\boldsymbol{u}\cdot\nabla\boldsymbol{\sigma} - g(\boldsymbol{u},\boldsymbol{\sigma})\right)$$
$$\frac{1}{2\eta_0}(1 + h(\boldsymbol{\sigma}))\cdot\boldsymbol{\sigma} = \mathbf{0} \text{ in } \Omega, t \in]0, t_f[,$$

where $g(\boldsymbol{u},\boldsymbol{\sigma}) = \boldsymbol{\sigma}\cdot\nabla\boldsymbol{u} - (\nabla\boldsymbol{u}^T)\cdot\boldsymbol{\sigma}$ and $\mathbf{T} = 2\beta\eta_0\nabla^s\boldsymbol{u} + \boldsymbol{\sigma}$.

Oldroyd-B
$h(\boldsymbol{\sigma}) = 0$

Giesekus
$h(\boldsymbol{\sigma}) = \frac{\epsilon\lambda}{\eta_p}\boldsymbol{\sigma}$

Phan-Thien-Tanner
$h(\boldsymbol{\sigma}) = \frac{\epsilon\lambda}{\eta_p}\text{tr}(\boldsymbol{\sigma})$

Introduction: The Weissemberg number

$$\frac{\lambda}{2\eta_0}\frac{\partial \boldsymbol{\sigma}}{\partial t} - (1-\beta)\nabla^s \boldsymbol{u} + \frac{\lambda}{2\eta_0}\left(\boldsymbol{u}\cdot\nabla\boldsymbol{\sigma} - g(\boldsymbol{u},\boldsymbol{\sigma})\right) + \frac{1}{2\eta_0}(1+h(\boldsymbol{\sigma}))\cdot\boldsymbol{\sigma} = \boldsymbol{0}$$

$$\mathrm{We} = \lambda\frac{U}{L}$$

- When We is small we have Newtonian viscosity fluid.
- When We > 1 the problems are interesting and extremally complicated.

Introduction: Stabilized formulation

Variational Multiscales Methods (VMS)

- Approximating the effect of the components of the solution of the continuous problem that cannot be resolved by the finite element mesh.
- Split the unknown as $\boldsymbol{U} = \boldsymbol{U}_h + \boldsymbol{U}'$, where $\boldsymbol{U}_h \in \boldsymbol{\mathcal{X}_h}$ and $\boldsymbol{U}' \in \boldsymbol{\mathcal{X}'}$.
  The spaces $\boldsymbol{\mathcal{X}_h}$ and $\boldsymbol{\mathcal{X}'}$ are such that $\boldsymbol{\mathcal{X}} = \boldsymbol{\mathcal{X}_h} \bigoplus \boldsymbol{\mathcal{X}'}$.

A standard problem, is exactly equivalent to:

$$\left(\mathbf{M}(\boldsymbol{U})\frac{\partial \boldsymbol{U}}{\partial t}, \boldsymbol{V}_h\right) + \langle \mathcal{L}(\boldsymbol{U}, \boldsymbol{U}), \boldsymbol{V}_h \rangle = \langle \boldsymbol{F}, \boldsymbol{V}_h \rangle \; \forall \boldsymbol{V}_h \in \boldsymbol{\mathcal{X}}_h,$$

$$\left(\mathbf{M}(\boldsymbol{U})\frac{\partial \boldsymbol{U}}{\partial t}, \boldsymbol{V}'\right) + \langle \mathcal{L}(\boldsymbol{U}, \boldsymbol{U}), \boldsymbol{V}' \rangle = \langle \boldsymbol{F}, \boldsymbol{V}' \rangle \; \forall \boldsymbol{V}' \in \boldsymbol{\mathcal{X}}',$$

Introduction: Stabilized formulation

VMS in the viscoelastic case

$$(\mathcal{D}_t(\boldsymbol{U}_h), \boldsymbol{V}_h) + B(\boldsymbol{u}_h; \boldsymbol{U}_h, \boldsymbol{V}_h) + \sum_K \langle \tilde{\boldsymbol{U}}, \mathcal{L}^*(\boldsymbol{u}_h; \boldsymbol{V}_h)\rangle_K = \langle \boldsymbol{f}, \boldsymbol{v}_h\rangle,$$

where

- $\mathcal{D}_t$ represents the temporal terms.
- B is the bilinear form of the variational problem.
- $\tilde{\boldsymbol{U}} = \boldsymbol{\alpha}\tilde{P}[\mathbf{F} - \mathcal{L}(\boldsymbol{u}_h; \boldsymbol{U}_h)]$ where $\tilde{P}$ is the L^2 projection onto the space of sub-grid scales, $\boldsymbol{\alpha}$ is a matrix computed within each element and $\mathcal{L}$ is the operator associated to the problem.
- $\mathcal{L}^*$ is the formal adjoint of the operator.

E. Castillo and R. Codina. Finite Element approximation of the viscoelastic flow problem: A non-residual based stabilized formulation. Computer and Fluids, 142 (2015)

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Thermal coupling: Introduction

Heat transfer processes

- Viscoelastic fluids have very advantageous properties for heat transfer and transport.
- As the Weissemberg number increases, the dynamics of viscoelastic fluid change. This turn out in a higher mixing capacity, with benefits in the heat transfer between the fluid and the pipe transporting it.
- Examples: Fire brigades water tanks, petroleum extraction, reducing the drag forces in submarines, chemical reactors.

Thermal coupling

Mathematical model

- The constitutive model used in literature for the coupling is the Phan Thien Tanner (PTT) model.
- Viscous dissipation is added in energy equation.
- Temperature dependency of the physical parameters λ and η_0.

Energy equation

$$\rho C_p \left(\frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta \right) = k \Delta \theta + \boldsymbol{\sigma} : \nabla^s \mathbf{u}$$

WLF function

$$\lambda(\theta) = \lambda(\theta_0) f(\theta),$$
$$\eta_0(\theta) = \eta_0(\theta_0) f(\theta)$$
$$f(\theta) = \exp\left[-\frac{c_1 \cdot (\theta - \theta_0)}{c_2 + (\theta - \theta_0)} \right]$$

Gerrit W.M. Peters, Frank P.T. Baaijens. Modelling of non-isothermal viscoelastic flows. Journal of non-Newtonians Fluid Mechanics, 68 (1997): 205-224

Thermal coupling: Fully system of equations

Momentum equation:

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} - \nabla \cdot \boldsymbol{\sigma} - 2\beta\eta_0(\theta)\nabla \cdot (\nabla^s \mathbf{u}) + \nabla p = \mathbf{f} \text{ in } \Omega, t \in]0, t_f[,$$

Continuity equation:

$$\nabla \cdot \mathbf{u} = 0 \text{ in } \Omega, t \in]0, t_f[,$$

Constitutive equation (PTT):

$$\frac{1}{2\eta_0(\theta)}\boldsymbol{\sigma} - (1-\beta)\nabla^s \mathbf{u} + \frac{\lambda(\theta)}{2\eta_0(\theta)}\left(\frac{\partial \boldsymbol{\sigma}}{\partial t} + \mathbf{u} \cdot \nabla \boldsymbol{\sigma} - \boldsymbol{\sigma} \cdot \nabla \mathbf{u} - (\nabla \mathbf{u}^T) \cdot \boldsymbol{\sigma}\right) + \frac{1}{2\eta_0(\theta)}\left(\epsilon \frac{\lambda(\theta)}{(1-\beta)\eta_0(\theta)} \mathrm{Tr}(\boldsymbol{\sigma})\boldsymbol{\sigma}\right) = \mathbf{0} \text{ in } \Omega, t \in]0, t_f[,$$

Energy equation:

$$\rho C_p \left(\frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta\right) - k\Delta\theta - \boldsymbol{\sigma} : \nabla^s \mathbf{u} = 0, \text{ in } \Omega, t \in]0, t_f[$$

Thermal coupling: Numerical Results

Algorithm employed is

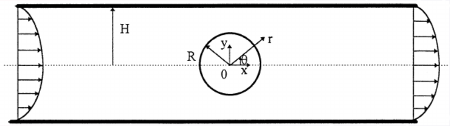
- iterative
- non-monolithic
- executed in a partitioner manner.

Time descretization scheme

Classical backward-difference (BDF) approximations.

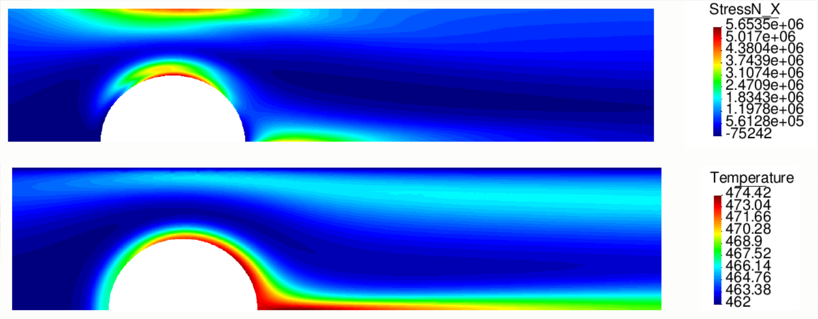
$$\delta_k g^{n+1} = \frac{1}{\gamma_k}\left(g^{n+1} - \sum_{i=0}^{k-1} \varphi_k^i g^{n-i} \right)$$

Validation: Flow around a cylinder



Scheme of the problem.

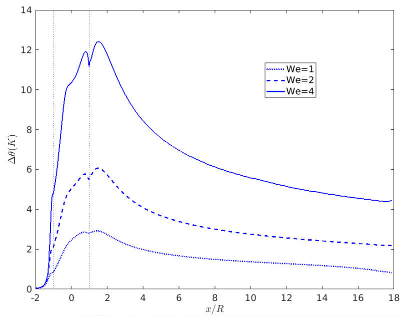
Thermal coupling: Validation



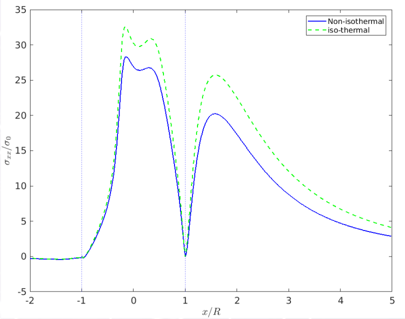
Distribution of temperature θ (below) and stress component σ_{xx} (top) around the cylinder for We=4.

Gerrit W.M. Peters, Frank P.T. Baaijens. Modelling of non-isothermal viscoelastic flows. Journal of non-Newtonians Fluid Mechanics, 68 (1997): 205-224

Thermal coupling: Validation



Temperature θ for We=1,2 and 4 as a function of x-coordinate.



Stress component σ_{xx}, We=4, in isothermal and non-isothermal case as a function of x-coordinate.

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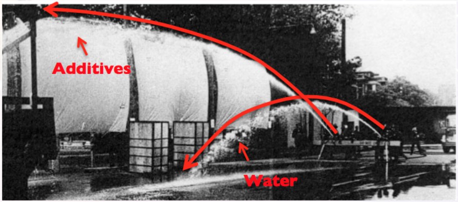
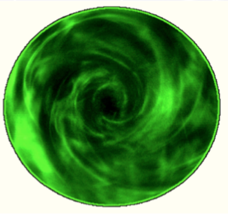
High Weissemberg Numbers: Turbulence

- Takes place when the elastic part of the fluid becomes relevant, that is, at high Weissemberg numbers.
- Transition to turbulence has been shown to take place earlier and at lower Reynolds number in viscoelastic solutions.
- The addition of long-chain polymers can help to reduce the turbulent friction reductions in the boundary layer.
- Examples: polymeric solutions and polymer casting.





The High Weissemberg Number Problem (HWNP)

- Computational rheology started in the early 1970s. Mostly finite-element methods for steady 2D flows.
- All methods, without exception, were found to **break down** at a “ustratingly low value” of the Weissenberg number.
- The reason for this breakdown has remained somewhat of a **mystery**. Evidence that it is a numerical phenomenon.
- The high-Weissenberg number problem has haunted computational rheology for over **30 years**.

Logarithmic conformation reformulation (LCR)

Reformulating constitutive laws

- Was proposed by Fattal and Kupferman.
- Seeks to treat the exponential growth of the elastic stresses when the elastic component becomes dominant.
- This allows to extend the range of Weissemberg numbers.

Logarithmic conformation reformulation (LCR)

- Physically-admissible conformation tensors must, by definition, be symmetric and positive-definite.

$$\boldsymbol{\sigma} = \frac{\eta_p}{\lambda_0}(\boldsymbol{\tau} - \mathbf{I}) \longrightarrow \boldsymbol{\tau} = \frac{\lambda_0 \boldsymbol{\sigma}}{\eta_p} + \mathbf{I}$$

- The conformation tensor is replaced by a new variable $\psi = \log(\boldsymbol{\tau})$.

So, inserting the descomposition in the equation, the constitutive law transforms into

$$\frac{1}{2\lambda_0}(\exp(\psi) - \mathbf{I}) - \nabla^s \boldsymbol{u} + \frac{\lambda}{2\lambda_0}\left(\boldsymbol{u} \cdot \nabla \exp\left(\psi\right)\right)$$

$$\frac{\lambda}{2\lambda_0} + \left(-\exp\left(\psi\right) \cdot \nabla \boldsymbol{u} - \left(\nabla \boldsymbol{u}\right)^T \cdot \exp\left(\psi\right) + 2\nabla^s \boldsymbol{u}\right) = \mathbf{0}$$

Logarithmic conformation reformulation (LCR)

Consequently, the new set of equations to be solved can be written as follows

$$
\begin{aligned}
-\frac{\eta_0(1-\beta)}{\lambda_0}\nabla\cdot\exp(\psi) - 2\beta\nabla\cdot(\nabla^s \boldsymbol{u}) + \rho\boldsymbol{u}\cdot\nabla\boldsymbol{u} + \nabla p &= \boldsymbol{f}, \\
\nabla\cdot\boldsymbol{u} &= 0, \\
\frac{1}{2\lambda_0}(\exp(\psi) - \mathbf{I}) - \nabla^s\boldsymbol{u} + \frac{\lambda}{2\lambda_0}\left(\boldsymbol{u}\cdot\nabla\exp\left(\psi\right)\right) + & \\
\frac{\lambda}{2\lambda_0}\left(-\exp\left(\psi\right)\cdot\nabla\boldsymbol{u} - \left(\nabla\boldsymbol{u}\right)^T\cdot\exp\left(\psi\right) + 2\nabla^s\boldsymbol{u}\right) &= \mathbf{0}
\end{aligned}
$$

Logarithmic conformation reformulation (LCR)

We have developed the linearization of LCR problem in order to design a stabilized formulation applying the Variational Multi-Scale method.

Difficulties in implementation

- Apart from the well-known non-linearities, a exponential function must be linearized.
- We have to be especially careful with convective term $\boldsymbol{u} \cdot \nabla \exp(\psi)$ and its linearization.
- The computational cost increases because of the calculation of the exponential.

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Summarizing

- Viscoelastic fluids have a wide range of applications in industry.
- Particularly, they have a higher mixing capacity and heat transfer properties.
- Simulating viscoelastic fluid flows at high Weissemberg numbers is currently one of the biggest challenges in computational rheology.

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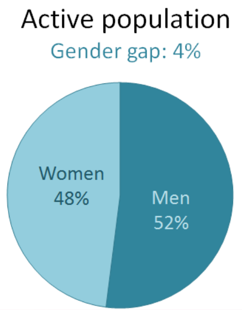
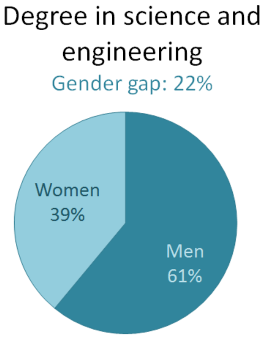
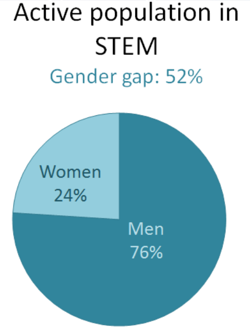
Women in science: statistics

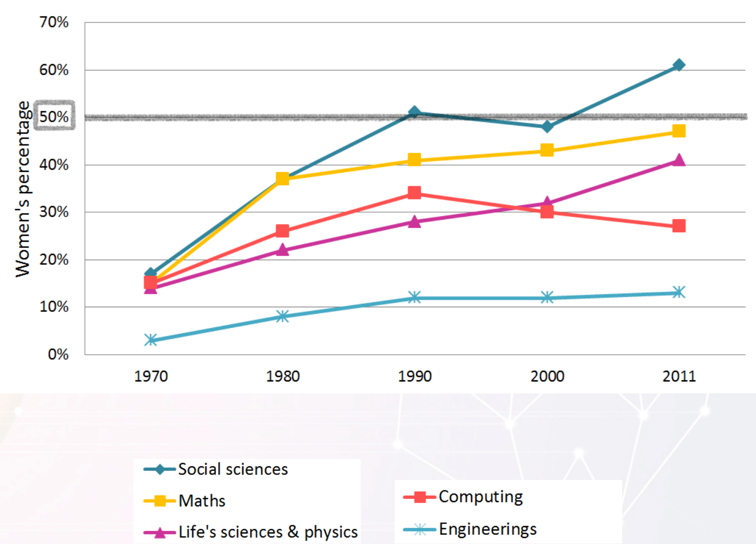
Statistics from USA until 2011 in fields of STEM (Science, Technology, Engineering and Mathematics).







Women in science: statistics



Women in science: engineering and mathematics









Thank you for your attention

Laura Moreno Martínez