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Thermal coupling simulations with a viscoelastic fluid flow

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Outline

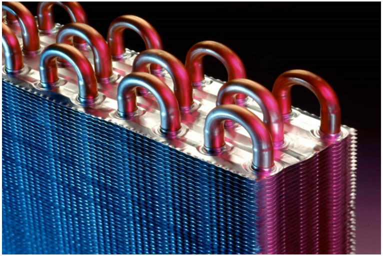
Introduction: Viscoelasticity

- 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: Heat properties

Viscoelastic fluids have very **advantageous properties** for heat transfer and transport.

- As the elasticity of the flow increases, the dynamics of viscoelastic fluid change, turning out in a **higher mixing capacity**.
- Transformation of large amounts of mechanical energy into **heat**; and consequently in a rising of the temperature material.
- **Examples**: Extruders, heat exchange, fire brigades water tanks, petroleum extraction, reducing the drag forces in submarines, chemical reactors.



Computing non-isothermal viscoelastic fluid flows

Viscoelastic materials

The stresses depends on:

1. Deformation and deformation history.
2. Temperature and temperature history.

$\Longrightarrow$ Temperature should be considered as an **independent variable** in the constitutive equations for the stress tensor.

Computing non-isothermal viscoelastic fluid flows

Viscoelastic problem

Temperature dependence of the linear viscoelastic properties by

THE PRINCIPLE OF TIME-TEMPERATURE SUPERPOSITION

If there is free convection flotation forces are considered too.

Temperature problem

In the energy equation now must be considered

- Mechanical power that is dissipated.
  $\Longrightarrow$ Viscous part
- Mechanical part that is accumulated as elastic energy.
  $\Longrightarrow$ Deformation part

The principle of time-temperature superposition (1)

Viscoelastic fluid flow equations

- Momentum equation:

$$\rho \frac{\partial \boldsymbol{u}}{\partial t} + \rho \boldsymbol{u} \cdot \nabla \boldsymbol{u} - \nabla \cdot \underbrace{\left(2\eta_s(\vartheta)\nabla^s \boldsymbol{u} + \boldsymbol{\sigma}\right)}_{\text{Deviatoric extra stress tensor}} + \nabla p = \boldsymbol{f} + \underbrace{\gamma \rho \boldsymbol{g}(\vartheta_0 - \vartheta)}_{\text{Only for free convection}}$$

- Continuity equation:

$$\nabla \cdot \boldsymbol{u} = 0$$

- Constitutive equation:

$$\frac{1}{2\eta_p(\vartheta)}(1 + \mathfrak{h}(\boldsymbol{\sigma})) \cdot \boldsymbol{\sigma} - \nabla^s \boldsymbol{u} + \frac{\lambda(\vartheta)}{2\eta_p(\vartheta)} \left(\frac{\partial \boldsymbol{\sigma}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{\sigma} \overbrace{- \boldsymbol{\sigma} \cdot \nabla \boldsymbol{u} + (\nabla \boldsymbol{u}^T) \cdot \boldsymbol{\sigma}}^{\text{Deformation terms}} \right) = \boldsymbol{0}$$

The principle of time-temperature superposition (2)

Two different models in literature:

1) Williams-Landel-Ferry

$$g_{\mathrm{wlf}}(\vartheta) = \exp\left[-\frac{c_a \cdot (\vartheta - \vartheta_0)}{c_b + (\vartheta - \vartheta_0)}\right]$$

where c_a and c_b are constants.

2) Arrhenius

$$g_{\mathrm{a}}(\vartheta) = \exp\left[c_r\left(\frac{1}{\vartheta} - \frac{1}{\vartheta_0}\right)\right]$$

where c_r is a constant parameter.

Relation between temperature and viscoelastic properties

$$\lambda(\vartheta) = \lambda(\vartheta_0) g(\vartheta)$$
$$\eta_0(\vartheta) = \eta_0(\vartheta_0) g(\vartheta)$$

Viscous dissipation

Energy equation

The heat source term is thus the classical one.

$$\rho C_p \left(\frac{\partial \vartheta}{\partial t} + \boldsymbol{u} \cdot \nabla \vartheta \right) - k \Delta \vartheta = \overbrace{\boldsymbol{\sigma} : \nabla^s \boldsymbol{u}}^{\text{Viscous dissipation}}$$

Viscous dissipation represents the **internal heat produced by internal work**: it means the contribution of the entropy elasticity.

Four relevant dimensionless numbers

Reynolds number

$$\mathrm{Re} = \frac{\rho U L}{\eta_0}$$

Inertial forces VS Viscous forces

Prandtl number

$$\mathrm{Pr} = \frac{\eta_0 C_p}{k_f}$$

Momentum VS Thermal diffusivity

Weissenberg number

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

Elastic forces VS Viscous forces

Brinkman number

$$\mathrm{Br} = \frac{\eta_0 U^2}{k_f(\vartheta_w - \vartheta_0)}$$

Inertial power VS Heat Conduction

The Weissenberg number and the Logarithmic Conformation Reformulation

$$\frac{1}{2\eta_p(\vartheta)}(1+\mathfrak{h}(\boldsymbol{\sigma}))\cdot\boldsymbol{\sigma} - \nabla^s \boldsymbol{u} + \frac{\lambda(\vartheta)}{2\eta_p(\vartheta)}\left(\frac{\partial\boldsymbol{\sigma}}{\partial t} + \overbrace{\boldsymbol{u}\cdot\nabla\boldsymbol{\sigma}}^{\text{convective term}} \overbrace{-\boldsymbol{\sigma}\cdot\nabla\boldsymbol{u} + (\nabla\boldsymbol{u}^T)\cdot\boldsymbol{\sigma}}^{\text{deformation terms}}\right) = \mathbf{0}$$

- We is small: Newtonian viscosity fluid.
- If We $>$ 1: problems are extremally complicated.

Weissenberg number

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

Logarithmic-Conformation Reformulation

$$\psi = \log(\boldsymbol{\tau}) = \log\left(\frac{\lambda_0\boldsymbol{\sigma}}{\eta_p} + \mathbf{I}\right) \longrightarrow \boldsymbol{\sigma} = \frac{\eta_p}{\lambda_0}(\exp(\psi) - \mathbf{I})$$

Change of variable

Thermal coupling using Logarithmic-Conformation Reformulation.

- Momentum equation:

$$-\nabla \cdot \frac{\eta_p(\vartheta)}{\lambda_0(\vartheta)} \exp(\psi) - 2\nabla \cdot \eta_s(\vartheta)(\nabla^s \boldsymbol{u}) + \rho \boldsymbol{u} \cdot \nabla \boldsymbol{u} + \nabla p = \boldsymbol{f}$$

- Continuity equation:

$$\nabla \cdot \boldsymbol{u} = 0$$

- Constitutive equation:

$$\frac{1}{2\lambda_0(\vartheta)}(\exp(\psi) - \boldsymbol{I}) \cdot (\mathfrak{h}(\exp(\psi)) + \boldsymbol{I}) - \nabla^{\mathrm{s}} \boldsymbol{u} + \frac{\lambda(\vartheta)}{2\lambda_0(\vartheta)} (\boldsymbol{u} \cdot \nabla \exp(\psi)) + \frac{\lambda(\vartheta)}{2\lambda_0(\vartheta)} \left(-\exp(\psi) \cdot \nabla \boldsymbol{u} - (\nabla \boldsymbol{u})^T \cdot \exp(\psi) + 2\nabla^s \boldsymbol{u} \right) = 0$$

- Energy equation:

$$\rho C_p \left(\frac{\partial \vartheta}{\partial t} + \boldsymbol{u} \cdot \nabla \vartheta \right) - k\Delta\vartheta = \left(\frac{\eta_p(\vartheta)}{\lambda_0(\vartheta)} \exp(\psi) - \mathbf{I} \right) : \nabla^s \boldsymbol{u}$$

Variational form of the problem (Standard formulation)

Finding $\boldsymbol{U} = [\boldsymbol{u}, p, \boldsymbol{\sigma}] \in \boldsymbol{\mathcal{X}} := \boldsymbol{\mathcal{V}} \times \mathcal{Q} \times \Upsilon$ such that

$$\mathcal{G}_{\text{std}}(\vartheta; \boldsymbol{U}, \boldsymbol{V}) + B_{\text{std}}(\boldsymbol{U}; \boldsymbol{U}, \boldsymbol{V}) = L_{\text{std}}(\boldsymbol{V}),$$

for all $\boldsymbol{V} \in \boldsymbol{\mathcal{X}}$, where

$$\begin{aligned}
\mathcal{G}_{\text{std}}(\hat{\vartheta}; \boldsymbol{U}, \boldsymbol{V}) =& \left(\rho \frac{\partial \boldsymbol{u}}{\partial t}, \boldsymbol{v}\right) + \left(\frac{\lambda(\hat{\vartheta})}{2\eta_0(\hat{\vartheta})} \frac{\partial \boldsymbol{\sigma}}{\partial t}, \chi\right) + \rho C_p \left(\frac{\partial \vartheta}{\partial t}, \xi\right), \\
B_{\text{std}}(\hat{\boldsymbol{U}}; \boldsymbol{U}, \boldsymbol{V}) =& 2(\eta_s(\hat{\vartheta})\nabla^s \boldsymbol{u}, \nabla^s \boldsymbol{v}) + \langle \rho \hat{\boldsymbol{u}} \cdot \nabla \boldsymbol{u}, \boldsymbol{v} \rangle + (\boldsymbol{\sigma}, \nabla^s \boldsymbol{v}) \\
& -(p, \nabla \cdot \boldsymbol{v}) + (q, \nabla \cdot \boldsymbol{u}) + \left(\frac{1}{2\eta_p(\hat{\vartheta})} (\mathbf{I} + \mathfrak{h}(\hat{\boldsymbol{\sigma}})) \cdot \boldsymbol{\sigma}, \chi\right) \\
& -(\nabla^s \boldsymbol{u}, \chi) + \left(\frac{\lambda(\hat{\vartheta})}{2\eta_p(\hat{\vartheta})} \left(\hat{\boldsymbol{u}} \cdot \nabla \boldsymbol{\sigma} - \boldsymbol{\sigma} \cdot \nabla \hat{\boldsymbol{u}} - (\nabla \hat{\boldsymbol{u}})^T \cdot \boldsymbol{\sigma}\right), \chi\right) \\
& + \rho C_p (\hat{\boldsymbol{u}} \cdot \nabla \vartheta, \xi) + (k \nabla \vartheta, \nabla \xi) - (\hat{\boldsymbol{\sigma}} : \nabla^s \hat{\boldsymbol{u}}, \xi), \\
L_{\text{std}}(\boldsymbol{V}) =& \langle \boldsymbol{f}, \boldsymbol{v} \rangle.
\end{aligned}$$

Discretization

Spatial discretization

Galerkin finite element approximation. Consists in finding $\boldsymbol{U}_h : (0, T) \longrightarrow \boldsymbol{\mathcal{X}}_h$,

$$\underbrace{\mathcal{G}(\vartheta_h; \boldsymbol{U}_h, \boldsymbol{V}_h)}_{\text{Temporal terms}} + \underbrace{B(\boldsymbol{U}_h; \boldsymbol{U}_h, \boldsymbol{V}_h)}_{\text{Bilinear form}} = L(\boldsymbol{V}_h),$$

for all $\boldsymbol{V}_h = [\boldsymbol{v}_h, q_h, \chi_h] \in \boldsymbol{\mathcal{X}}_h$

Time discretization

Monolithic time discretization. BDF1 and BDF2 schemes have been employed in the work to reach a stationary solution.

Variational Multiscale Methods (VMS)

- To approximate the components of the continuous problem solution that cannot be resolved by the finite element mesh.
- Split the unknowns as $\boldsymbol{U} = \underbrace{\boldsymbol{U}_h}_{\in \boldsymbol{\mathcal{X}_h}} + \underbrace{\tilde{\boldsymbol{U}}}_{\in \tilde{\boldsymbol{\mathcal{X}}}}$ and $\boldsymbol{\mathcal{X}} = \boldsymbol{\mathcal{X}_h} \bigoplus \tilde{\boldsymbol{\mathcal{X}}}$.

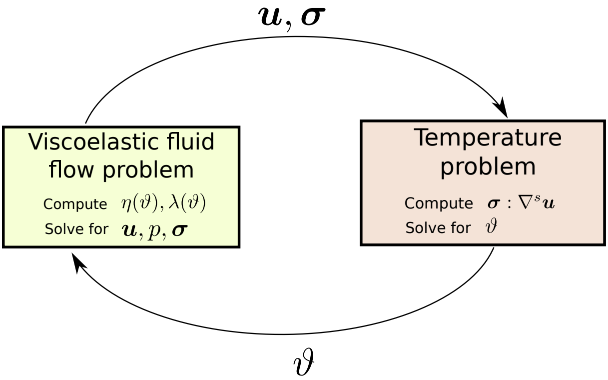
$$\tilde{\boldsymbol{U}} = \boldsymbol{\alpha}\tilde{P}[\mathbf{F} - \mathcal{D}_t(\boldsymbol{U}_h) - \mathcal{L}(\boldsymbol{U}_h; \boldsymbol{U}_h)]$$

Sub-grid scale

$$\underbrace{\mathcal{G}(\vartheta_h; \boldsymbol{U}_h, \boldsymbol{V}_h) + B(\boldsymbol{U}_h; \boldsymbol{U}_h, \boldsymbol{V}_h)}_{\text{Galerkin terms}} + \underbrace{\sum_K \langle \tilde{\boldsymbol{U}}, \underbrace{\mathcal{L}^*(\boldsymbol{U}_h; \boldsymbol{V}_h)}_{\text{adjoint operator of } \mathcal{L}} \rangle_K}_{\text{Stabilization terms}} = L(\boldsymbol{V}_h)$$

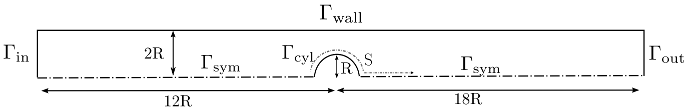
- $\tilde{P}$ is the L^2 projection onto the space of sub-grid scales,
- $\boldsymbol{\alpha}$ is a matrix computed within each element,
- $\mathcal{L}$ is the operator associated to the problem.

Algorithm



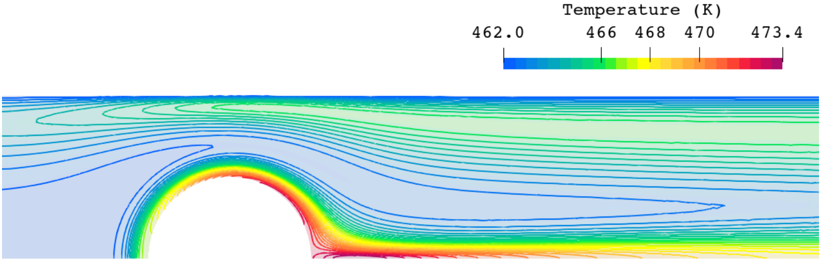
The algorithm is iterative for coupling but monolithic for the fluid flow problem.
The parameters are continuously updated.

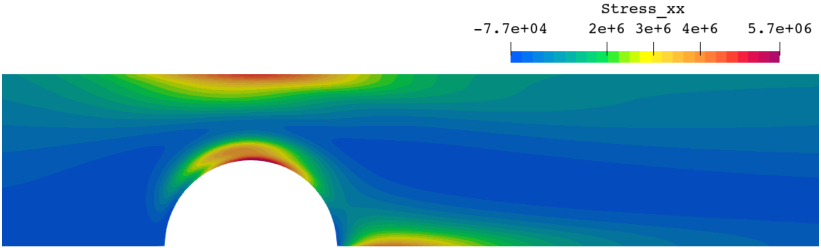
Flow past a cylinder: Set up



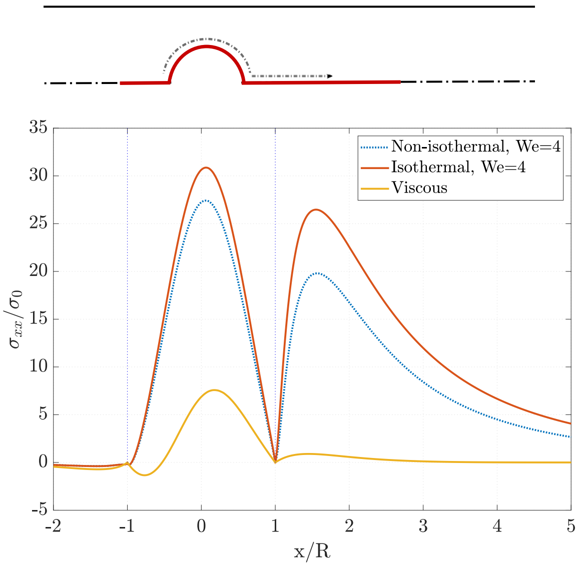
- The computational domain: R=0.03
- The boundary conditions of the problem are:
  - The inflow velocity is $u_x = 1.2$m/s and $u_y = 0$.
  - Symmetry conditions are prescribed along the axis.
  - For the outflow boundary the velocity is free in both components.
  - Non-slip conditions are set in the wall of the cylinder and on the top wall.
  - Temperature ϑ_0 is imposed at inlet and on the top wall.
- The viscoelastic fluid parameters are: $\rho = 921\text{kg}\cdot\text{m}^{-3}$, $\beta = 0.5$ and $\eta_0(\vartheta_0) = 10^4$, $\lambda(\vartheta_0) = 0.1s$. WLF function.
- The temperature parameters are: ϑ_0=462K, $C_p = 1.5\text{kJ}(\text{kg}\cdot\text{K}^{-1})$ and $k_f = 0.17\text{W}(\text{m}\cdot K^{-1})$.
- Dimensionless numbers: Re=0.0033, We $\in \{0, 1, 2, 3, 4\}$, Pe=Pr Re $>> 1$.
- Spatial discretization: Mesh of triangles with 58591 elements and 36174 nodes.

Flow past a cylinder: Distribution of temperature and stresses

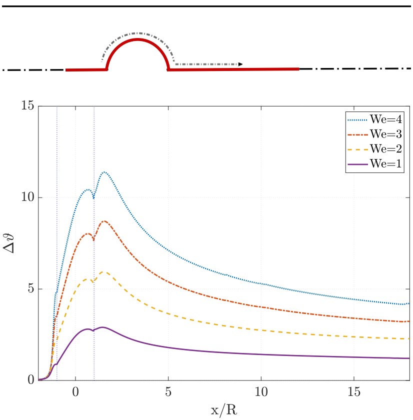




Flow past a cylinder: Comparison of stresses



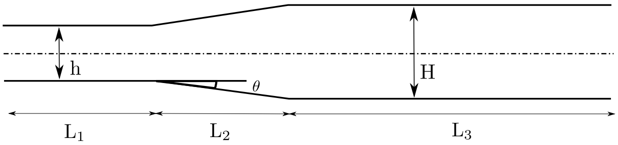
Flow past a cylinder: Comparison of temperatures



Two main conclusions:

- **Reduction of stresses** when thermal coupling is considered.
- **Increment of temperature** when the Weissenberg number increase.

1:3 Expansion. Set up



- The computational domain: h=0.1; H=0.3; L_1=60h; L_3=120h; $\theta = 60^\circ$
- The boundary conditions of the problem are:
  - The inflow velocity is imposed u_x (different for each case) and $u_y = 0$.
  - For the outflow boundary the velocity is free in both components.
  - Non-slip conditions are set on walls.
  - Temperature ϑ_0=563.5K is imposed on walls and as initial condition.
  - Temperature $\vartheta_i = 463.5$K is imposed on the inlet.
- The viscoelastic fluid parameters are: $\rho = 1226 \text{kg} \cdot \text{m}^{-3}$, $\beta = 0.5$ and $\eta_0(\vartheta_0) = 4.07$, $\lambda(\vartheta_0)$ different for each case. Arrhenius function.
- The temperature parameters are: ϑ_0=463.5K, C_p and k_f also is specific of each case.
- Dimensionless numbers: Re $\in [0, 200]$, We $\in [0, 3]$, Pr $\in [0, 25]$, Br $\in [0, 100]$.
- Spatial discretization: Structured mesh of bilinear elements.

Newtonian case. Validation.

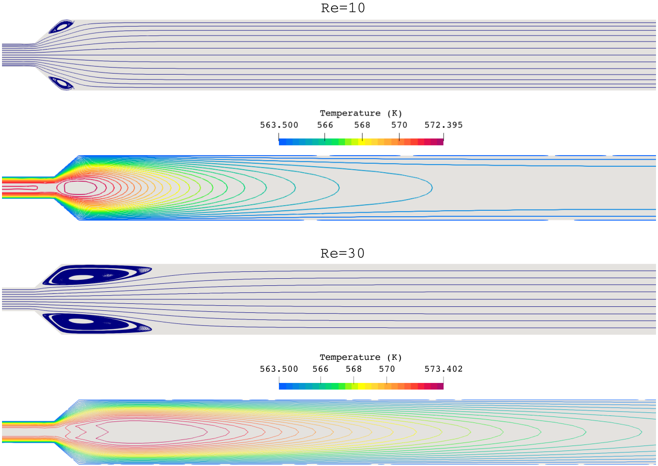


Figure: Streamlines and temperature contours for $\mathrm{Re} = 10$ and 30.

Newtonian case. Validation.

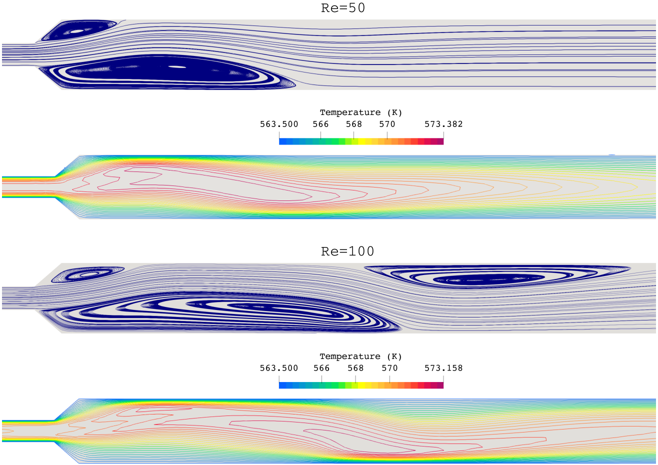
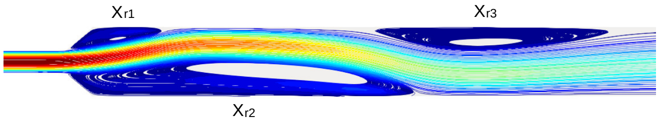
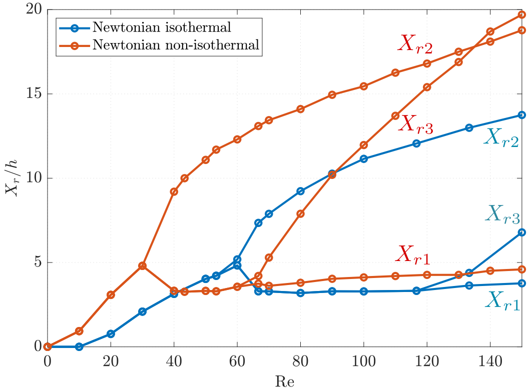


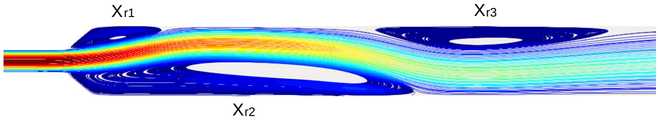
Figure: Streamlines and temperature contours for $\mathrm{Re} = 50$ and 100.

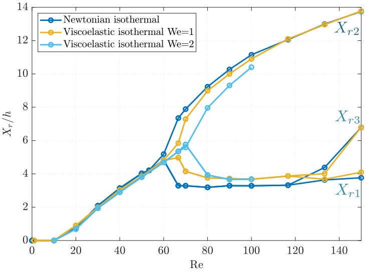
1. Reynolds number study

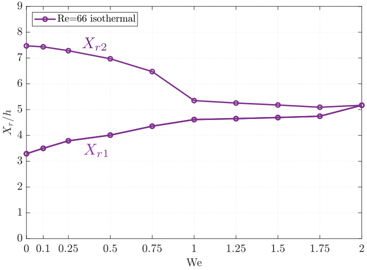




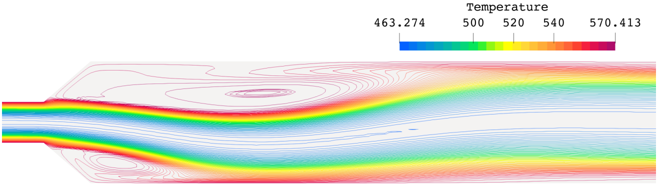
2. Weissenberg number study

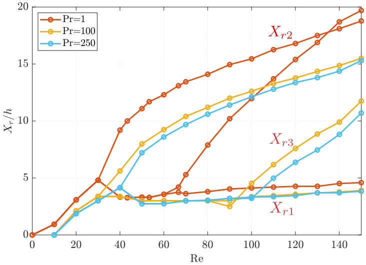


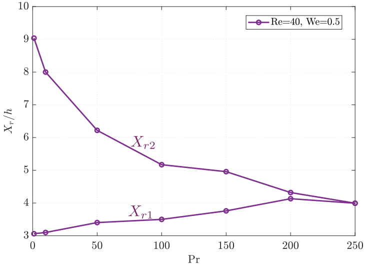




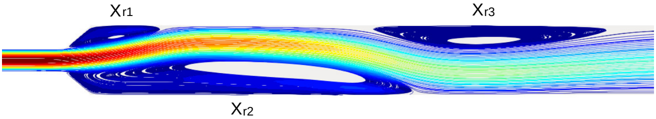
3. Prandtl number study

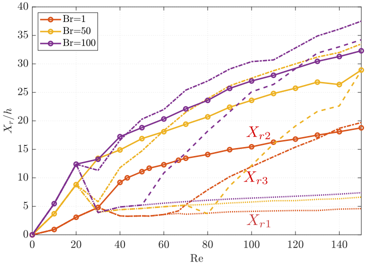


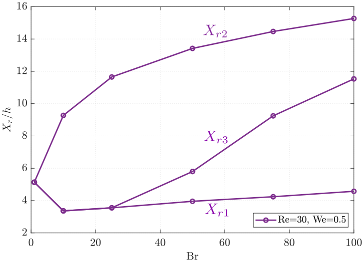




4. Brinkman number study







Conclusions

- Coupling with temperature is established through a temperature dependence with **viscoelastic parameters**, and adding the **viscous dissipation** term in the energy equation.
- We need **four** dimensionless numbers to define the problem.
- Viscous dissipation effect is very significant in two benchmark studied, due to implies an **increment of the temperature**.
- Temperature increment as function of the **Weissenberg number** while the stresses reduces when temperature increases.
- For the 1:3 expansion benchmark, the coupling with the temperature implies that
  - The influence of other parameters has been explored varying the **Prandtl** number and the **Brinkman** too apart from Reynolds and Weissenberg numbers.
  - As a general trend and for the models considered herein, the flow is **more stable** for low Re, high We, low Br and high Pr.

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Thank you for your attention!!

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