Implementation of integral viscoelastic constitutive models in OpenFOAM® computational library

M. S. B. de Araujo[1], C. Fernandes [2], L.L. Ferrás[2], Željko Tukovic[3], Hrvoje Jasak[4] and J. Miguel Nóbrega[2]

[1] *Universidade Federal do Pará - Instituto de Ciências Exatas e Naturais,*
Faculdade de Matemática. - 66075-110 - Belém, PA – Brazil

[2] *Institute for Polymers and Composites/i3N, University of Minho,*
Campus of Azurém, 4800-058 Guimarães, Portugal

[3] *Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb,*
Croatia

[4] *Wikki Ltd., London, United Kingdom*

July 11, 2015

Outline

- Motivation
- Objective
- Numerical Modelling Code
- Code Verification
  - Couette Flow Startup Flow (Analytical Solution)
  - Couette Flow Ramped Wall Velocity
  - Couette Flow Constant Wall Velocity
  - 4:1 Abrupt Planar Contraction
- Conclusions

Motivation

Differential viscoelastic flow solvers[1]

Multi mode constitutive models		
UCM	(L,E, Feta) PTT	FENE-(P,CR)
Oldroyd-B	Giesekus	(S,D) XPP
White Metzner	Leonov	DCPP

No integral model implemented

---

[1] JL Favero et al. (Computer Aided Chemical Engineering, 2009, 2010 / Journal of non-Newtonian Fluid Mechanics, 2010 / Computers & Chemical Engineering, 2010

Objective

Implement and verify an Integral Viscoelastic flow solver in OpenFOAM® using a methodology based on the Deformation Fields approach [2]

---

[2] M.A. Hulsen, E.A.J.F. Peters, B.H.A.A. van den Brule, J. Non-Newtonian Fluid Mech. 98, (2001)

Numerical Modelling Code

Governing equations

- Conservation of Mass:

$$\nabla \cdot \mathbf{u} = 0 \tag{1}$$

- Conservation of Linear Momentum:

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau} \tag{2}$$

- Constitutive Equation:

$$\boldsymbol{\tau}(t) = \int_{-\infty}^{t} M(t-t')\ f\left[\mathbf{B}(t,t')\right] dt' \tag{3}$$

Numerical Modelling Code

Integral Viscoelastic Constitutive Equation

$$\boldsymbol{\tau}(t) = \int_{-\infty}^{t} M(t-t')\ f\left[\mathbf{B}(t,t')\right] dt'$$

$$M(t-t') = \sum_i \frac{a_i}{\lambda_i} \exp\left(-\frac{t-t'}{\lambda_i}\right) \tag{4}$$

$$\mathbf{B}(t,t')] = \begin{cases} \mathbf{B}(t,t') & , \quad UCM \;\; integral \\ \dfrac{\alpha}{\alpha - 3 + \beta I_1 + (1-\beta) I_2}\mathbf{B}(t,t') & , \quad K-BKZ \;\; model \end{cases} \tag{5}$$

$$I_1 = tr(\mathbf{B}) \qquad\qquad I_2 = \frac{1}{2}\left[(tr\,\mathbf{B})^2 - tr\left(\mathbf{B}^2\right)\right]$$

Numerical Modelling Code

Stress Tensor Field Calculation

- Define cutoff time (s_{max}) and number of **deformation fields**(n_f);
- At each time step $t = t_n$:
  1. Update velocity and pressure fields (PISO)
  2. Transport all the previously created deformation fields $\mathbf{B}(t_{n-1}, t'_k),\ k = 0, 1, \cdots, n_f - 1$, according to

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot (\mathbf{uB}) - \left[(\nabla \mathbf{u})^T \cdot \mathbf{B} + \mathbf{B} \cdot \nabla \mathbf{u} \right] = \mathbf{0} \qquad (6)$$

  3. create a new deformation field ($\mathbf{B}(t_n, t_n) = \mathbf{I}$)
  4. If required redistribute/interpolate the deformation fields[3]
  5. Compute the stress field:

$$\boldsymbol{\tau}(t_n) = \int_{-\infty}^{t_c} M(t_n - t')\ f\,[\mathbf{B}(t_n, t_c)]\, dt' + \int_{t_c}^{t_n} M(t_n - t')$$

where $t_c = \max\{0, t_n - s_{max}\}$

---

[3] Araujo, M.S.B - PhD Thesis,ICMC-USP, 2006 / M.F. Tomé et al., Journal of Computational Physics, 227 (2008) 4207-4243

Stress Tensor Field Calculation

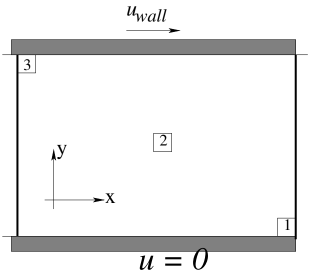
In order to calculate the second integral in right hand side the interval $[t_c,\ t_n]$ is divided to perform numerical integration.

$$\int_{t_c}^{t_n} M(t_n - t')\ f\left[\mathbf{B}(t_n, t')\right] dt' = \sum_k \int_{t'_{2k}}^{t'_{2k+2}} M(t_n - t')\ f\left[\mathbf{B}(t_n, t')\right] dt'$$

There are a number of ways to divide the integration domain. For now we use equally spaced subintervals.
A second order scheme is employed to solve the integrals.

Code Verification

Couette Flow - UCM - Imposed Velocity and Pressure Fields

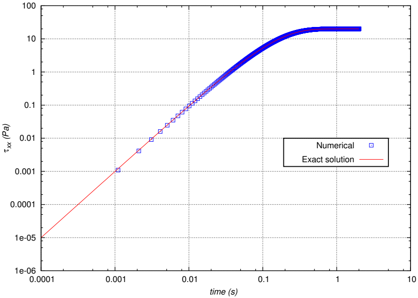


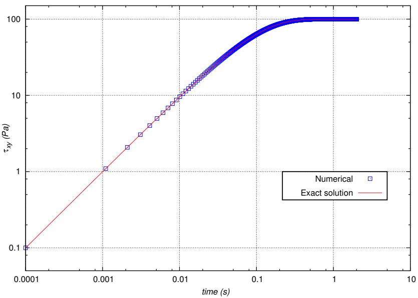
$$u(t) = \begin{cases} 0 & , t < 0 \\ \dot{\gamma} y & , t \geq 0 \end{cases}$$

$$\tau_{xx}(t) = 2a\dot{\gamma}^2\lambda^2 \left[1 - \exp\left(-\frac{t}{\lambda}\right)\left(1 + \frac{t}{\lambda}\right)\right]$$

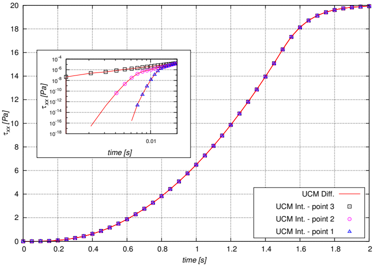
$$\tau_{xy}(t) = a\dot{\gamma}\lambda\left[1 - \exp\left(-\frac{t}{\lambda}\right)\right]$$

Couette Flow - UCM - Imposed Velocity

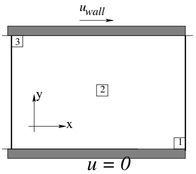


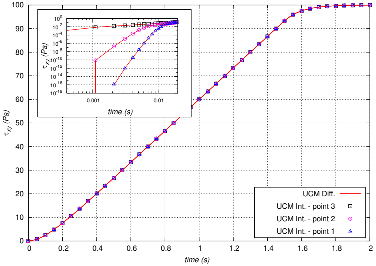


Couette Flow - UCM - Ramped Wall Velocity

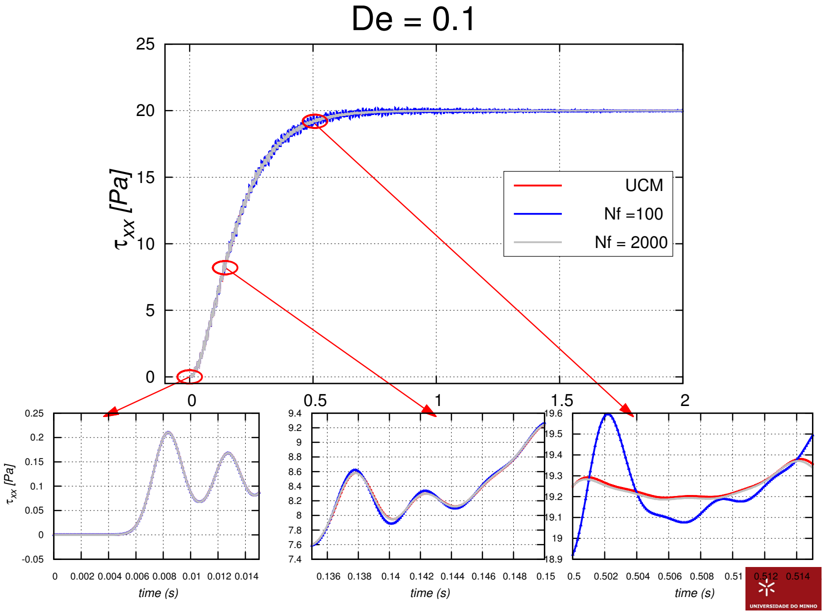


$$u(t) = \begin{cases} u_0 \dfrac{t}{t_f} & , 0 \leq t < t_f \\ u_0 & , t \geq t_f \end{cases}$$



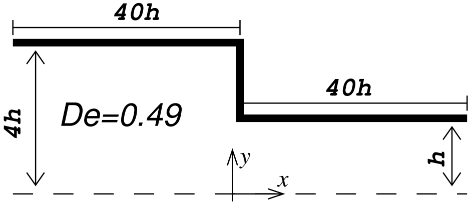


Couette Flow – UCM – Constant Wall Velocity



4:1 Abrupt Planar Contraction – K- BKZ

Solution of 5% wt. polyisobutylene (PIB) in Tetradecane(C14)[4,5]



$s_{max} = 1.5s$

$n_f = 150$

k	λ_k (s)	a_k (Pa)
1	0.6855	0.058352
2	0.1396	1.664756
3	0.0389	14.560411
4	0.0059	99.152542

$\alpha = 10$

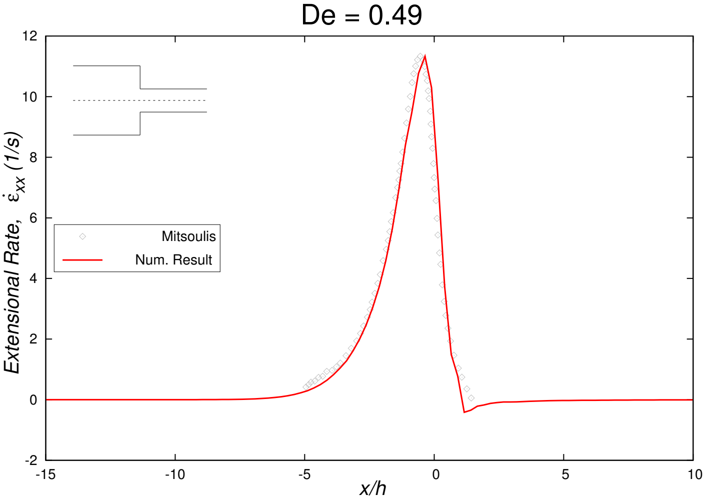
$\beta = 0.7$

---

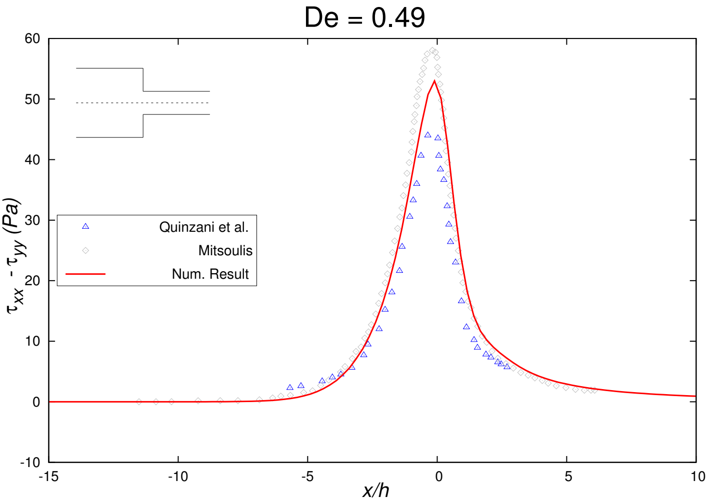
[4] LM Quinzani, RC Armstrong, RA Brown, Journal non-Newtonian Fluid Mechanics, 52, 1994

[5] E Mitsoulis, Journal of Rheology, 37, 1993

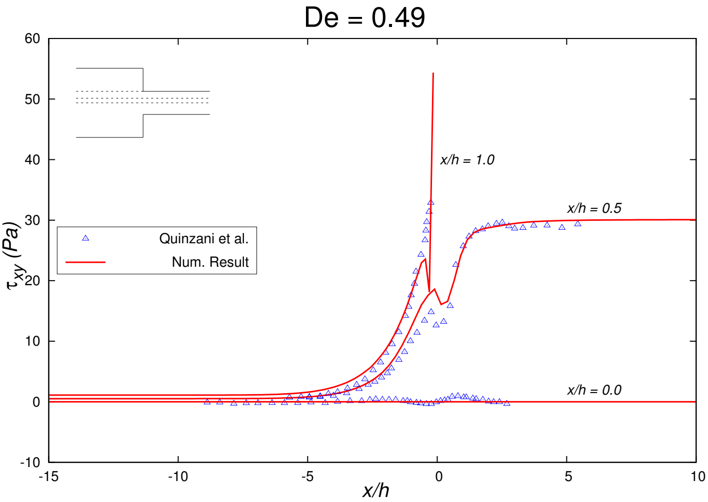
4:1 Abrupt Planar Contraction – K- BKZ



4:1 Abrupt Planar Contraction – K- BKZ



4:1 Abrupt Planar Contraction – K- BKZ



Conclusions

- A new solver that can handle integral viscoelastic constitutive equations was implemented in OpenFOAM®
- The implementation was verified with some case studies
- Additional verification/assessment studies are required
  - $\mathbf{B}$ distribution
  - n_f
  - S_{max}

Thanks!