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Viscoelastic flow analysis using the software OpenFOAM and differential constitutive equations

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ABSTRACT

Viscoelastic fluids are of great importance in many industrial sectors, such as in food and synthetic polymers industries. The rheological response of viscoelastic fluids is quite complex, including combination of viscous and elastic effects and non-linear phenomena. This work presents a numerical methodology based on the split-stress tensor approach and the concept of equilibrium stress tensor to treat high Weissenberg number problems using any differential constitutive equations. The proposed methodology was implemented in a new computational fluid dynamics (CFD) tool and consists of a viscoelastic fluid module included in the OpenFOAM, a flexible open source CFD package. Oldroyd-B/UCM, Giesekus, Phan-Thien–Tanner (PTT), Finitely Extensible Nonlinear Elastic (FENE-P and FENE-CR), and Pom–Pom based constitutive equations were implemented, in single and multimode forms. The proposed methodology was evaluated by comparing its predictions with experimental and numerical data from the literature for the analysis of a planar 4:1 contraction flow, showing to be stable and efficient.

1. Introduction

Processing operations involving viscoelastic melts, solutions, or suspensions are usually the key step in the definition of the characteristics and quality of the finished products in polymer and food industries. Therefore, understanding and modeling viscoelastic flows is of fundamental importance in these industrial sectors. The rheological response of viscoelastic fluids is quite complex, including combination of non-linear viscous and elastic effects, such as strain rate dependent viscosity, presence of normal stress differences in shear flows, relaxation phenomena, and memory effects, including die swell [1,2].

Numerous studies on the numerical analysis of viscoelastic flows using one or more non-linear differential models can be found in literature. A common difficulty in all these works, regardless of the discretization method (finite element, finite differences, or finite volume), iterative solution method, or constitutive equations used, is the so-called 'High Weissenberg Number Problem' (HWNP). The HWNP consists in the difficulty of achieving convergence at high Weissenberg (*We*) or Deborah (*De*) numbers, where the dimensionless numbers *We* and *De* are ratios between a characteristic relaxation time of the polymer and a characteristic flow time. The higher the Weissenberg (or Deborah) number, the more pronounced the elastic effect. In the attempt of solving the HWNP or minimizing its effects, many strategies have been proposed, including special interpolations schemes [3,4] and specific numerical methodologies coupling momentum and constitutive viscoelastic equations [5–8].

Another relevant aspect regarding the analysis of viscoelastic flows is the development of software specifically designed for this purpose. Despite the extensive literature on viscoelastic behavior modeling and viscoelastic flow simulation, most of commercial packages intended to be applied to the analysis of polymeric flows and polymer processing operations, such as extrusion and injection molding, are actually limited to the description of purely viscous non-Newtonian phenomena. Development and use of software with viscoelastic flow analysis capability is still carried out almost exclusively in academic environments, for specific applications.

According to this scenario the insertion of a viscoelastic fluid flow solver in a widely recognized CFD (*computational fluid dynamics*) package is a relevant matter, since it would bring to viscoelastic fluid flow analysis field the main features of CFD packages, which include the possibility of analyzing complex geometries using unstructured and non-orthogonal meshes, moving meshes, large variety of interpolation schemes and solvers for the linear discretized system, data processing parallelization among others benefits.

Being a well-tested and widely used free open source CFD package, with the intrinsic advantages of being writen in the C++ object-oriented language, in this context the OpenFOAM (*Open*

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Source Field Operation and Manipulation) package [9,10] appears as a promising tool for this kind of development. The flexibility to deal with unstructured and moving meshes and to implement complex mathematical models are some of its attractive features.

Therefore, the goal of this work was to create a general purpose viscoelastic fluid flow solver to be used in OpenFOAM CFD package. For this, a numerical methodology based on the split-stress tensor approach [6–8,11] and on the concept of equilibrium stress tensor was developed to treat the HWNP and deal with any differential constitutive equations. The so-called viscoelasticFluidFoam solver was evaluated by comparing its predictions with experimental and numerical data from the literature for the analysis of a planar 4:1 contraction flow.

2. Methodology

In this section the mathematical formulation and the main aspects related to the viscoelasticFluidFoam solver are presented. The case study used to evaluate the solver is also presented.

2.1. Mathematical model

The governing equations for isothermal incompressible flows of viscoelastic fluids are the mass conservation (continuity):

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

and momentum conservation:

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

together with a constitutive equation to describe the relation between the stress and deformation rate for the fluid of interest. In the above equations ρ is the density of the fluid, $\mathbf{u}$ the velocity vector, p the pressure, and $\boldsymbol{\tau}$ the stress tensor.

The stress tensor can be divided into a Newtonian solvent contribution $\boldsymbol{\tau}_S$ and an elastic polymeric contribution (or extra elastic stress tensor) $\boldsymbol{\tau}_P$:

$$\boldsymbol{\tau} = \boldsymbol{\tau}_S + \boldsymbol{\tau}_P \tag{3}$$

with $\boldsymbol{\tau}_S$ defined by:

$$\boldsymbol{\tau}_S = 2\eta_S \mathbf{D} \tag{4}$$

where η_S is the solvent viscosity and $\mathbf{D}$ is the deformation rate tensor given by:

$$\mathbf{D} = \frac{1}{2}(\nabla \mathbf{u} + [\nabla \mathbf{u}]^T) \tag{5}$$

The $\boldsymbol{\tau}_P$ is a symmetric tensor obtained as the sum of the contributions of the individual relaxation modes:

$$\boldsymbol{\tau}_P = \sum_{K=1}^{n} \boldsymbol{\tau}_{P_K} \tag{6}$$

with the expression for $\boldsymbol{\tau}_{P_K}$ depending on the viscoelastic constitutive equation.

The differential constitutive equations used in this work are presented in Table 1. Since all these equations are well known and extensively used in the literature, the expressions for the upper convected ($\overset{\nabla}{\boldsymbol{\tau}}_{P_K}$), lower convected ($\overset{\Delta}{\mathbf{S}}_{P_K}$) and Gordon–Schowalter ($\overset{\square}{\boldsymbol{\tau}}_{P_K}$) derivatives, and the meaning of the parameters which appear in the models of Table 1 are not shown here. The expressions for the mentioned derivatives can be found in classic rheology books [1,2], while for detailed information about these models and their parameters the reader is suggested to refer to [12–22].

2.2. Pressure–velocity and momentum–stress coupling and tensorial viscosity

Velocity–pressure coupling was accomplished by segregated methods, in which the continuity equation is used to formulate an equation for the pressure, using a semi-discretized form of Eq. (2)[23]. The resulting equation set is solved by a decoupled approach, using iterative algorithms with under-relaxation, such as SIMPLE [24].

Regarding momentum–stress coupling and numerical stabilization in the solution of the momentum equation, the strategy employed consists of decomposing the viscoelastic stress into an implicit component aligned with $\mathbf{D}$, defined on the basis of a tensorial viscosity $\boldsymbol{\eta}_\mathbf{T}$, and an explicit correction:

$$\nabla \cdot \boldsymbol{\tau} \approx \nabla \cdot (\boldsymbol{\eta}_\mathbf{T} \cdot \nabla \mathbf{u}) + \nabla \cdot \boldsymbol{\tau}_{\mathrm{corr}} \tag{7}$$

Addtionally, the stress transport models were written in the following generic form:

$$\frac{\partial}{\partial t}\boldsymbol{\tau} + \nabla \cdot (\mathbf{u}\boldsymbol{\tau}) = \frac{\boldsymbol{\tau}^* - \boldsymbol{\tau}}{\lambda} \tag{8}$$

This equation describes transport of $\boldsymbol{\tau}$ in space by the velocity field, with simultaneous relaxation towards the equilibrium value $\boldsymbol{\tau}^*$, where $\boldsymbol{\tau}^*$ is the stress state achieved in the absence of transport effects and λ is the relaxation time scale. It is possible to achieve this form irrespective of the specific model used. For multi-mode versions of the stress models, each mode will present its own equilibrium stress, which can be combined in the usual manner.

From Eq. (8), one can clearly see that $\boldsymbol{\tau}^*$ must be related to the local value of $\mathbf{D}$, specifically because it excludes the effects of relaxation and transport. Furthermore, the magnitude of $\boldsymbol{\eta}_\mathbf{T}$, that is related with $\mathbf{D}$ and $\boldsymbol{\tau}^*$, will be considerably higher than the Newtonian viscosity (Eq. (4)), whose effective contribution is generally not significant for realistic non-linear flows of polymeric melts. This higher magnitude of $\boldsymbol{\eta}_\mathbf{T}$ represents a key aspect in the methodology used in this work, since the stability in the numerical solution of the momentum equation is strongly dependent on the magnitude of the implicit Laplacian-like term.

A consistent and model-independent expression for $\boldsymbol{\eta}_\mathbf{T}$ may be obtained based on the definition:

$$\boldsymbol{\tau}^* = \boldsymbol{\eta}_\mathbf{T} \cdot \mathbf{D} \tag{9}$$

from which:

$$\boldsymbol{\eta}_\mathbf{T} = \boldsymbol{\tau}^* \cdot \mathbf{D}^{-1} \tag{10}$$

For cases where $det(\mathbf{D}) = 0$ (implying that a velocity gradient is a singular tensor), $\boldsymbol{\eta}_\mathbf{T} = \mathbf{0}$ or $\boldsymbol{\eta}_\mathbf{T} = \eta_P \mathbf{I}$ are adequate choices. For multi-mode versions of the stress models, components of $\boldsymbol{\eta}_\mathbf{T}$ can be summed up in the same manner as constituent stress tensors.

In this formulation, the momentum equation was implemented in the following form:

$$\frac{\partial(\rho\,\mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}\,\mathbf{u}) - \nabla \cdot (\boldsymbol{\eta}_\mathbf{T} \cdot \nabla \mathbf{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau}_{\mathrm{corr}} \tag{11}$$

where the dominant Laplacian-like term, $\nabla \cdot (\boldsymbol{\eta}_\mathbf{T} \cdot \nabla \mathbf{u})$ guarantees stability through implicit treatment, while the correction term $\nabla \cdot \boldsymbol{\tau}_{\mathrm{corr}}$ is simply calculated as the difference between the divergence of the instantaneous stress $\boldsymbol{\tau}$ and the implicit counterpart, i.e, the term $\nabla \cdot (\boldsymbol{\eta}_\mathbf{T} \cdot \nabla \mathbf{u})$. Note that $\nabla \cdot \boldsymbol{\tau}_{\mathrm{corr}}$ also carries the relaxation component $(\boldsymbol{\tau} - \boldsymbol{\tau}^*)$, which tends to zero over the relaxation time-scale λ.

For segregated approaches, one can further simplify the tensorial Laplacian-like $\nabla \cdot (\boldsymbol{\eta}_\mathbf{T} \cdot \nabla \mathbf{u})$, using a decomposition into a spherical component of $\boldsymbol{\eta}_\mathbf{T}$, with the deviatoric part being absorbed into $\boldsymbol{\tau}_{\mathrm{corr}}$.